A Study of Extremal Trees for the ABS Index Based on Total Domination Number and Its Predictive Power in Molecular Modeling

Manuel, M. [1] and Parthiban A.* [1]

[1]*Department of Mathematics, School of Advanced Sciences,*
Vellore Institute of Technology, Vellore, 632014, Tamil Nadu, India

E-mail: parthiban.a@vit.ac.in
*Corresponding author

Abstract

The atom-bond sum-connectivity (ABS) index is a refined topological descriptor derived from several well-known chemical graph indices, including the sum-connectivity index (SCI), the atom-bond connectivity index (ABC) and the Randić index (R). In recent years, exploring the interplay between topological indices and graph parameters has become a prominent area of research. This paper establishes a new lower bound for the ABS index of trees in terms of their total domination number. Extremal trees that achieve this bound are characterized, providing insight into structural configurations that optimize the index under domination constraints. To evaluate the practical applicability of the theoretical results, a set of carboxylic acid molecules is examined using linear regression models. The predictive power of the ABS index in capturing key physicochemical properties is assessed and compared against its variants$-ABC$, SCI and R indices. The analysis reveals strong correlations between these indices and molecular properties, underscoring their effectiveness in chemical informatics. Overall, this work integrates graph theory and molecular chemistry, demonstrating the value of topological indices in understanding and modeling chemical behavior.

M. Manuel and A. Parthiban

Malaysian J. Math. Sci. 20(1): 21–42(2026) 21 - 42

1   Introduction

For a connected, simple graph $G = (V(G), E(G))$, let $\alpha_1 \alpha_2$ represent an edge connecting the vertices α_1 and α_2, where $\alpha_1, \alpha_2 \in V(G)$. Define $N(\alpha) = \{\beta \in V \mid \alpha\beta \in E\}$ as the set of neighbors of any $\alpha \in V$, whose cardinality is the degree of α, represented as d_α in G. A tree $\mathscr{T}$ is a connected graph without cycles. A pendant vertex α in $\mathscr{T}$ is such that $d_\alpha = 1$. Let $\mathscr{T} - \{\alpha_1, \dots, \alpha_k\}$ refer to the tree obtained by removing the vertices $\alpha_1, \dots, \alpha_k$ from $\mathscr{T}$. The symbols S_p and P_p, respectively, represent the star and the path on p vertices. The diameter d represents the greatest distance between any pair of pendant vertices in a tree. Refer to [25] for definitions of other notations and terminologies not covered here.

Graph theory has offered chemists numerous valuable tools, with topological indices being particularly significant. These indices serve as quantitative descriptors of molecules, based on the unique topological properties of their molecular graphs. Ali et al. [3] introduced the atom-bond sum-connectivity index of a graph as a novel variation of several well-known chemical topological indices, including the atom-bond connectivity index [10], the sum-connectivity index [11] and the Randić index [20]. These indices are defined in Table 1.

Table 1: List of topological indices used in the study.

Atom-bond sum-connectivity index	$ABS(G) = \displaystyle\sum_{\alpha\beta \in E(G)} \sqrt{\dfrac{d_\alpha + d_\beta - 2}{d_\alpha + d_\beta}}.$
Atom-bond connectivity index	$ABC(G) = \displaystyle\sum_{\alpha\beta \in E(G)} \sqrt{\dfrac{d_\alpha + d_\beta - 2}{d_\alpha . d_\beta}}.$
Sum-connectivity index	$SCI(G) = \displaystyle\sum_{\alpha\beta \in E(G)} \dfrac{1}{\sqrt{d_\alpha + d_\beta}}.$
Randić index	$R(G) = \displaystyle\sum_{\alpha\beta \in E(G)} \dfrac{1}{\sqrt{d_\alpha . d_\beta}}.$

A dominating set (DS) $\mathscr{D} \subseteq V(G)$ is a subset where each vertex in $V(G) \setminus \mathscr{D}$ has at least one neighbor in $\mathscr{D}$. The domination number, $\gamma(G)$ is the smallest possible size of such a set. If the set $\mathscr{D}$ satisfies $N(\mathscr{D}) = V(G)$, then $\mathscr{D}$ is a total dominating set (TDS). The minimum size of a TDS is called the total domination number, $\gamma_t(G)$ [9]. Extensive research has been carried out on domination across various graph classes [12], with numerous variants thoroughly investigated in the literature [1]. Refer to the survey [14] for additional information on topics pertaining to domination.

The relationship between various domination parameters and topological indices in graphs has long attracted research interest and remains an active area of study [16]. Indices such as the Randić [7], Zagreb [8], geometric-arithmetic [5] and Sombor [22] indices have been investigated in relation to the domination number. Likewise, recent studies have investigated the minimum Randić index [2], maximum Randić index [13], geometric-arithmetic index [6], Sombor index [23] and their relationships with the total domination number. Zhang et al. [28] explored extremal problems on ABS indices for trees with given matching or domination numbers. Building on previous studies, this article establishes a new lower bound for the ABS index of trees in terms of their total domination number. Extremal trees that attain this bound are characterized, offering

insights into the structural properties of graphs that optimize topological indices with respect to domination parameters.

To validate the effectiveness of the derived bound, a set of 17 carboxylic acid structures is analyzed using a linear regression model. Furthermore, a comparative study is conducted on variations of the ABS index-namely, the ABC, SCI and R indices-to examine their correlations with selected physicochemical properties of these acids. This analysis aims to highlight the utility of these indices in capturing molecular behavior and properties. The integration of graph-theoretical concepts with chemical informatics emphasizes the practical applicability of topological tools in advancing chemical research.

2 Preliminary Concepts

Let $\mathscr{T}_{p,\gamma_t}$ denote the set of p-vertex trees with total domination number γ_t. Denote $\zeta_1(\alpha, \beta) = \sqrt{\dfrac{\alpha + \beta - 2}{\alpha + \beta}}$. The following results can be readily observed.

Lemma 2.1. [3] *For a p-vertex tree $\mathscr{T}$ with $p \geq 3$, it holds that,*

$$\frac{(p-1)\sqrt{p-2}}{\sqrt{p}} = ABS(S_p) \geq ABS(\mathscr{T}) \geq ABS(P_p) = \frac{(p-3)}{\sqrt{2}} + \frac{2}{\sqrt{3}}.$$

Lemma 2.2. [28] *Let* $h_1(z) = \sqrt{\dfrac{z - c_1}{z - c_1 + 2}} - \sqrt{\dfrac{z - c_2}{z - c_2 + 2}}$ *with* $z \geq c_2 \geq c_1 \geq 0$*, then, $h_1(z)$ is positive and decreasing in $c_2 \leq z < \infty$.*

Lemma 2.3. [28] *Let* $h_2(z) = (z - c_1)\sqrt{\dfrac{z - c_1}{z - c_1 + 2}} - (z - c_2)\sqrt{\dfrac{z - c_2}{z - c_2 + 2}}$ *with* $z \geq c_2 \geq c_1 \geq 0$*, then, $h_2(z)$ is positive and increasing in $c_2 \leq z < \infty$.*

A family of trees $\mathscr{G}$ is constructed as follows [6]: The path of order $4k$ is included in $\mathscr{G}$ for $k \geq 1$. If $\mathscr{T} \in \mathscr{G}$ and there are two vertices $\alpha_1, \alpha_2 \in V(\mathscr{T})$ such that $N(\alpha_1) = \{\theta_1, \alpha_2\}$, $N(\alpha_2) = \{\alpha_1, \theta_2\}$, $d_{\theta_1} = d_{\theta_2} = 2$ and α_1, α_2 are in a minimum TDS in $\mathscr{T}$, then two paths P_{4l_1+1} and P_{4l_2+1} with $4l_1 + 1$ and $4l_2 + 1$ vertices, respectively, are considered. The tree $\mathscr{T}'$, constructed as,

$$V(\mathscr{T}') = V(\mathscr{T}) \cup V(P_{4l_1+1}) \cup V(P_{4l_2+1}),$$

and

$$E(\mathscr{T}') = E(\mathscr{T}) \cup E(P_{4l_1+1}) \cup E(P_{4l_2+1}) \cup \{\alpha_1\eta_1, \alpha_2\eta_2\},$$

is in $\mathscr{G}$, where η_1 and η_2 are pendant vertices in P_{4l_1+1} and P_{4l_2+1}, respectively (see Figure 1, with dark vertices denoting the members of a minimum TDS).

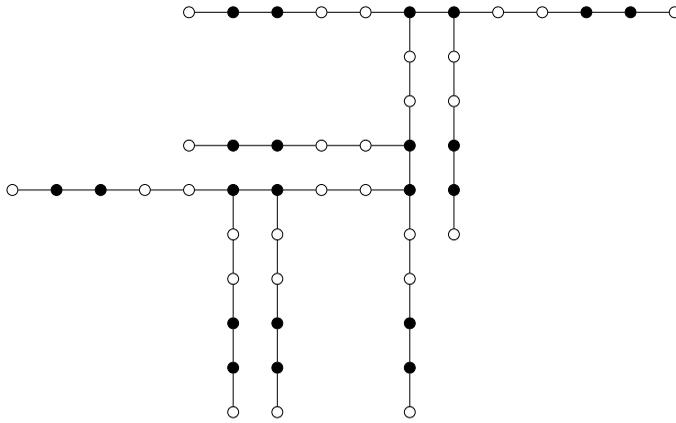M. Manuel and A. Parthiban

Malaysian J. Math. Sci. 20(1): 21–42(2026) 21 - 42

Figure 1: A sample tree from the family $\mathscr{G}$.

Define $\mathscr{G}_{p,\gamma_t}$ as the set of all $\mathscr{T} \in \mathscr{G}$ having p vertices and total domination number γ_t. Denote,

$$\xi_{p,\gamma_t} = (p - 2\gamma_t)\left(\frac{1 + \sqrt{2}}{\sqrt{6}} + \frac{2\sqrt{3}}{\sqrt{5}} - \frac{5}{2\sqrt{2}}\right) + \frac{2\gamma_t}{\sqrt{2}} + \frac{2}{\sqrt{3}} - \frac{3}{\sqrt{2}}.$$

Lemma 2.4. $ABS(\mathscr{T}) = \xi_{p(\mathscr{T}),\gamma_t(\mathscr{T})}$ *for each* $\mathscr{T} \in \mathscr{G}_{p,\gamma_t}$.

Proof. Let l_q represent the number of vertices that have a degree of q. For $\mathscr{T} \in \mathscr{G}_{p,\gamma_t}$,

$$p = l_1 + l_2 + l_3,$$
$$2(p - 1) = l_1 + 2l_2 + 3l_3,$$
$$\gamma_t = l_3 + \frac{p - 3l_3}{2}.$$

Hence, $l_1 = p - 2\gamma_t + 2$, $l_2 = 4\gamma_t - p - 2$ and $l_3 = p - 2\gamma_t$. Applying these equations to the definitions of $\mathscr{G}_{p,\gamma_t}$ and the ABS index,

$$ABS(\mathscr{T}) = l_1\zeta_1(2,1) + 2l_3\zeta_1(3,2) + \frac{l_3}{2}\zeta_1(3,3) + \left(p - 1 - l_1 - \frac{5}{2}l_3\right)\zeta_1(2,2)$$

$$= (p - 2\gamma_t + 2)\left(\frac{1}{\sqrt{3}}\right) + 2(p - 2\gamma_t)\left(\sqrt{\frac{3}{5}}\right) + \left(\frac{p - 2\gamma_t}{2}\right)\left(\sqrt{\frac{4}{6}}\right)$$

$$+ \left(-\frac{5}{2}p + 7\gamma_t - 3\right)\left(\sqrt{\frac{2}{4}}\right)$$

$$= (p - 2\gamma_t)\left(\frac{\sqrt{2} + 1}{\sqrt{6}} + \frac{2\sqrt{3}}{\sqrt{5}} - \frac{5}{2\sqrt{2}}\right) + \frac{2\gamma_t}{\sqrt{2}} + \frac{2}{\sqrt{3}} - \frac{3}{\sqrt{2}}$$

$$= \xi_{p(\mathscr{T}),\gamma_t(\mathscr{T})}.$$

$\square$

3   Lower Bound for the ABS Index on $\mathscr{T}_{p,\gamma_t}$

Lemma 3.1. *Let* $g(a) = \dfrac{(a-1)\sqrt{a-2}}{\sqrt{a}} - (a-4)\left(\dfrac{1+\sqrt{2}}{\sqrt{6}} + \dfrac{2\sqrt{3}}{\sqrt{5}} - \dfrac{5}{2\sqrt{2}}\right) - \dfrac{1}{\sqrt{2}} - \dfrac{2}{\sqrt{3}}$. *Then,*
$g(a) > 0$ *whenever* $a \geq 5$.

Proof.

$$g'(a) = \frac{a^2 - a - 1}{a^{\frac{3}{2}}\sqrt{a-2}} - 0.7670 > 0, \quad \forall\, a \geq 5.$$

Thus, $g(a) \geq g(5) = \dfrac{4\sqrt{3}}{\sqrt{5}} - \left(\dfrac{1+\sqrt{2}}{\sqrt{6}} + \dfrac{2\sqrt{3}}{\sqrt{5}} - \dfrac{5}{2\sqrt{2}}\right) - \dfrac{1}{\sqrt{2}} - \dfrac{2}{\sqrt{3}} = 0.4696 > 0.$ $\square$

Theorem 3.1 presents $\xi_{p(\mathscr{T}),\gamma_t(\mathscr{T})}$ as a lower bound for $ABS(\mathscr{T})$ on $\mathscr{T}_{p,\gamma_t}$ and identifies the extremal trees.

Theorem 3.1. *For* $\mathscr{T} \in \mathscr{T}_{p,\gamma_t}$, *it holds that* $ABS(\mathscr{T}) \geq \xi_{p(\mathscr{T}),\gamma_t(\mathscr{T})}$, *with equality arising if and only if* $\mathscr{T} \in \mathscr{G}_{p,\gamma_t}$.

Proof. When $p = 3$, $ABS(P_3) = \dfrac{2}{\sqrt{3}} > \xi_{3,2}$.

If $p = 4$, $ABS(S_4) = \dfrac{3}{\sqrt{2}} > \xi_{4,2}$, $ABS(P_4) = \dfrac{1}{\sqrt{2}} + \dfrac{2}{\sqrt{3}} = \xi_{4,2}$.

A tree $\mathscr{T}$ in $\mathscr{T}_{p,\gamma_t}$; $p \geq 5$ is examined, presuming that all trees of order $p - 1$ meet the inequality. For a diameter $\alpha_1, \alpha_2, \ldots, \alpha_{d+1}$ of $\mathscr{T}$, $\mathscr{T} \cong S_p$ whenever $d = 2$ and $ABS(S_p) - \xi_{p,2} > 0$, the result holds (by Lemma 3.1). Assume $d \geq 3$. Denote,

$$
\begin{aligned}
d_{\alpha_2} &= j, \; N(\alpha_2) = \{\alpha_1, \alpha_3, \omega_1, \ldots, \omega_{j-2}\}, \\
d_{\alpha_3} &= k, \; N(\alpha_3) = \{\alpha_2, \alpha_4, \beta_1, \ldots, \beta_{k-2}\}, \\
d_{\alpha_4} &= l, \; N(\alpha_4) = \{\alpha_3, \alpha_5, \eta_1, \ldots, \eta_{l-2}\}, \\
d_{\alpha_5} &= q, \; N(\alpha_5) = \{\alpha_4, \alpha_6, \theta_1, \ldots, \theta_{q-2}\}, \quad \text{and} \\
d_{\alpha_6} &= r, \; N(\alpha_6) = \{\alpha_5, \alpha_7, z_1, \ldots, z_{r-2}\}.
\end{aligned}
$$

Then, the following claims are validated, leading to an analysis of various cases. Lemmas 2.2 and 2.3 are employed for simplifications.

  Claim 1: Let, $d_{\alpha_1} = d_{\omega_1} = \cdots = d_{\omega_{j-2}} = 1$ and $d_{\alpha_3} \geq 2$. If $j \geq 3$, then, $ABS(\mathscr{T}) > \xi_{p,\gamma_t}$ (see
      Figure 2).

Proof. Let, $\mathscr{T}_1 = \mathscr{T} - \{\alpha_1\}$. Then,

$$ABS(\mathscr{T}) = ABS(\mathscr{T}_1) - (j-2)\zeta_1(j-1,1) + (j-1)\zeta_1(j,1) + \zeta_1(d_{\alpha_3},j) - \zeta_1(d_{\alpha_3},j-1)$$

$$\geq \xi_{p-1,\gamma_t} + \sqrt{\frac{j-1}{j+1}} + (j-2)\left(\sqrt{\frac{j-1}{j+1}} - \sqrt{\frac{j-2}{j}}\right)$$

$$+ \left(\sqrt{\frac{j+d_{\alpha_3}-2}{j+d_{\alpha_3}}} - \sqrt{\frac{j+d_{\alpha_3}-3}{j+d_{\alpha_3}-1}}\right)$$

$$> \xi_{p,\gamma_t} - \left(\frac{1+\sqrt{2}}{\sqrt{6}} + \frac{2\sqrt{3}}{\sqrt{5}} - \frac{5}{2\sqrt{2}}\right) + \sqrt{\frac{2}{4}} + \left(\sqrt{\frac{2}{4}} - \sqrt{\frac{1}{3}}\right) + \left(\sqrt{\frac{3}{5}} - \sqrt{\frac{2}{4}}\right)$$

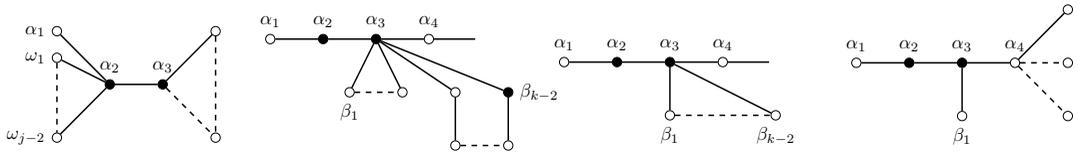$$= \xi_{p,\gamma_t} + 0.1373 > \xi_{p,\gamma_t}.$$

$\square$

Figure 2: Sample trees for Claims 1, 2, 3 and 4, respectively.

Claim 2: Let, $d_{\alpha_1} = 1$, $d_{\alpha_2} = 2$, $d_{\beta_m} \leq 2$, $m \in \{1, 2, \ldots, k-2\}$. If there is a minimum TDS $\mathscr{D}$ satisfying $|\mathscr{D} \cap N(\alpha_3)| \geq 2$, then, $ABS(\mathscr{T}) > \xi_{p,\gamma_t}$ (see Figure 2).

Proof. While $d_{\alpha_3} = 2$, take $\mathscr{T}_2 = \mathscr{T} - \{\alpha_1\}$. Then,

$$ABS(\mathscr{T}) = ABS(\mathscr{T}_2) - \zeta_1(k,1) + \zeta_1(k,2) + \zeta_1(2,1)$$

$$\geq \xi_{p-1,\gamma_t-1} + \sqrt{\frac{k}{k+2}} - \sqrt{\frac{k-1}{k+1}} + \frac{1}{\sqrt{3}}$$

$$> \xi_{p,\gamma_t} + \frac{1+\sqrt{2}}{\sqrt{6}} + \frac{2\sqrt{3}}{\sqrt{5}} - \frac{5}{2\sqrt{2}} - \frac{2}{\sqrt{2}} + \sqrt{\frac{2}{4}} - \sqrt{\frac{1}{3}} + \sqrt{\frac{1}{3}}$$

$$= \xi_{p,\gamma_t} + 0.0599 > \xi_{p,\gamma_t}.$$

While $d_{\alpha_3} \geq 3$, take $\mathscr{T}_3 = \mathscr{T} - \{\alpha_1, \alpha_2\}$. Then,

$$ABS(\mathscr{T}) = ABS(\mathscr{T}_3) - \zeta_1(d_{\beta_{k-2}}, k-1) + \zeta_1(d_{\beta_{k-2}}, k) + \zeta_1(k,2) + \zeta_1(2,1)$$

$$+ \sum_{m=1}^{k-2} [\zeta_1(d_{\beta_m}, k) - \zeta_1(d_{\beta_m}, k-1)]$$

$$\geq \xi_{p-2,\gamma_t-1} + \zeta_1(3,2) + \zeta_1(2,1) + \zeta_1(3,2) - \zeta_1(2,2)$$

$$> \xi_{p,\gamma_t} - \frac{2}{\sqrt{2}} + \sqrt{\frac{3}{5}} - \sqrt{\frac{2}{4}} + \sqrt{\frac{3}{5}} + \sqrt{\frac{1}{3}}$$

$$= \xi_{p,\gamma_t} + 0.0052 > \xi_{p,\gamma_t}.$$

$\square$

Claim 3: Suppose that, $d_{\alpha_1} = 1, d_{\alpha_2} = 2, d_{\alpha_3} \geq 4$. If $d_{\beta_1} = \cdots = d_{\beta_{k-2}} = 1$, then, $ABS(\mathcal{T}) > \xi_{p,\gamma_t}$ (see Figure 2).

Proof. Let, $\mathcal{T}_4 = \mathcal{T} - \{\beta_{k-2}\}$. Then,

$$
\begin{aligned}
ABS(\mathcal{T}) &= ABS(\mathcal{T}_4) - \zeta_1(k-1,2) - (k-3)\zeta_1(k-1,1) - \zeta_1(d_{\alpha_4}, k-1) \\
&\quad + \zeta_1(k,2) + (k-2)\zeta_1(k,1) + \zeta_1(d_{\alpha_4}, k) \\
&> \xi_{p-1,\gamma_t} + \zeta_1(4,2) - \zeta_1(3,2) + \zeta_1(4,1) + \zeta_1(4,1) - \zeta_1(3,1) \\
&= \xi_{p,\gamma_t} - \left(\frac{1+\sqrt{2}}{\sqrt{6}} + \frac{2\sqrt{3}}{\sqrt{5}} - \frac{5}{2\sqrt{2}} \right) + \sqrt{\frac{4}{6}} - \sqrt{\frac{3}{5}} + 2\sqrt{\frac{3}{5}} - \sqrt{\frac{2}{4}} \\
&= \xi_{p,\gamma_t} + 0.1169 > \xi_{p,\gamma_t}.
\end{aligned}
$$

$\square$

Claim 4: Suppose that, $d_{\alpha_1} = 1, d_{\alpha_2} = 2, d_{\alpha_3} = 3, d_{\alpha_4} \leq 3$ with $d_{\beta_1} = 1$. Then, $ABS(\mathcal{T}) > \xi_{p,\gamma_t}$ (see Figure 2).

Proof. Consider $\mathcal{T}_5 = \mathcal{T} - \{\beta_1\}$ and as in Claim 3,

$$
\begin{aligned}
ABS(\mathcal{T}) &= ABS(\mathcal{T}_5) - \zeta_1(2,2) + \zeta_1(3,2) + \zeta_1(3,1) + \zeta_1(d_{\alpha_4}, 3) - \zeta_1(d_{\alpha_4}, 2) \\
&\geq \xi_{p-1,\gamma_t} - \zeta_1(2,2) + \zeta_1(3,2) + \zeta_1(3,3) - \zeta_1(3,2) + \zeta_1(3,1) \\
&= \xi_{p,\gamma_t} - \left(\frac{1+\sqrt{2}}{\sqrt{6}} + \frac{2\sqrt{3}}{\sqrt{5}} - \frac{5}{2\sqrt{2}} \right) + \sqrt{\frac{4}{6}} - \sqrt{\frac{3}{5}} + \sqrt{\frac{3}{5}} - \sqrt{\frac{2}{4}} + \sqrt{\frac{2}{4}} \\
&= \xi_{p,\gamma_t} + 0.0495 > \xi_{p,\gamma_t}.
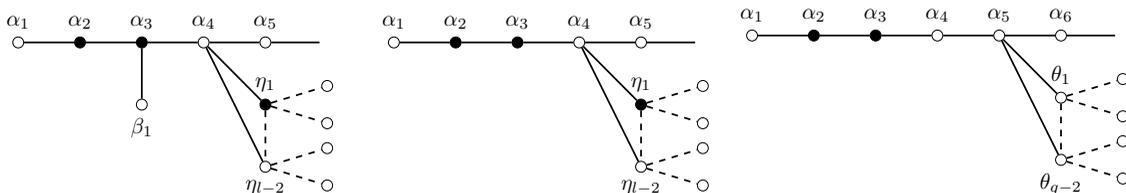\end{aligned}
$$

$\square$

Figure 3: Sample trees for Claims 5, 6 and 7, respectively.

Claim 5: Suppose that, $d_{\alpha_1} = 1, d_{\alpha_2} = 2, d_{\alpha_3} = 3, d_{\alpha_4} \geq 4$ with $d_{\beta_1} = 1$. If $|N(\alpha_4) \cap \mathcal{D}| \geq 2$, then, $ABS(\mathcal{T}) > \xi_{p,\gamma_t}$ (see Figure 3).

Proof. Let, $\mathcal{T}_6 = \mathcal{T} - \{\alpha_1, \alpha_2, \alpha_3, \beta_1\}$. Then,

$$
\begin{aligned}
ABS(\mathcal{T}) &= ABS(\mathcal{T}_6) - \zeta_1(d_{\alpha_5}, l-1) + \zeta_1(d_{\alpha_5}, l) + \zeta_1(l,3) + \zeta_1(3,2) + \zeta_1(3,1) \\
&\quad + \zeta_1(2,1) + \sum_{m=1}^{l-2} [\zeta_1(d_{\eta_m}, l) - \zeta_1(d_{\eta_m}, l-1)] \\
&> \xi_{p-4,\gamma_t-2} + \zeta_1(4,3) + \zeta_1(3,2) + \zeta_1(3,1) + \zeta_1(2,1) \\
&= \xi_{p,\gamma_t} - \frac{4}{\sqrt{2}} + \sqrt{\frac{5}{7}} + \sqrt{\frac{2}{4}} + \sqrt{\frac{3}{5}} + \sqrt{\frac{1}{3}} \\
&= \xi_{p,\gamma_t} + 0.0758 > \xi_{p,\gamma_t}.
\end{aligned}
$$

$\square$

Claim 6: Suppose that, $d_{\alpha_1} = 1$, $d_{\alpha_2} = d_{\alpha_3} = 2$, $d_{\alpha_4} \geq 3$. If $|N(\alpha_4) \cap \mathscr{D}| \geq 2$ with $d_{\eta_m} \leq 4$, $m \in \{1, \ldots, l-2\}$, then, $ABS(\mathscr{T}) > \xi_{p,\gamma_t}$ (see Figure 3).

Proof. Let $\mathscr{T}_7 = \mathscr{T} - \{\alpha_1, \alpha_2, \alpha_3\}$. Then,

$$ABS(\mathscr{T}) = ABS(\mathscr{T}_7) - \zeta_1(d_{\alpha_5}, l-1) + \zeta_1(d_{\alpha_5}, l) + \zeta_1(l, 2) + \zeta_1(2, 2) + \zeta_1(2, 1)$$
$$+ \sum_{m=1}^{l-2} [\zeta_1(d_{\eta_m}, l) - \zeta_1(d_{\eta_m}, l-1)]$$
$$> \xi_{p-3,\gamma_t-2} + \zeta_1(4, 3) - \zeta_1(4, 2) + \zeta_1(3, 2) + \zeta_1(2, 2) + \zeta_1(2, 1)$$
$$= \xi_{p,\gamma_t} + \frac{1+\sqrt{2}}{\sqrt{6}} + \frac{2\sqrt{3}}{\sqrt{5}} - \frac{5}{2\sqrt{2}} - \frac{4}{\sqrt{2}} + \sqrt{\frac{5}{7}} - \sqrt{\frac{4}{6}} + \sqrt{\frac{3}{5}} + \sqrt{\frac{2}{4}} + \sqrt{\frac{1}{3}}$$
$$= \xi_{p,\gamma_t} + 0.0263 > \xi_{p,\gamma_t}.$$

$\square$

Claim 7: Suppose that, $d_{\alpha_1} = 1$, $d_{\alpha_2} = d_{\alpha_3} = d_{\alpha_4} = 2$, $d_{\alpha_5} \geq 4$ with $d_{\theta_m} \leq 4$, $m \in \{1, \ldots, q-2\}$, then $ABS(\mathscr{T}) > \xi_{p,\gamma_t}$ (see Figure 3).

Proof. Assume $\alpha_4 \notin \mathscr{D}$. Let $\mathscr{T}_8 = \mathscr{T} - \{\alpha_1, \alpha_2, \alpha_3, \alpha_4\}$. Then,

$$ABS(\mathscr{T}) = ABS(\mathscr{T}_8) - \zeta_1(d_{\alpha_6}, q-1) + \zeta_1(d_{\alpha_6}, q) + \zeta_1(q, 2) + 2\zeta_1(2, 2) + \zeta_1(2, 1)$$
$$+ \sum_{m=1}^{q-2} [\zeta_1(d_{\theta_m}, q) - \zeta_1(d_{\theta_m}, q-1)]$$
$$> \xi_{p-4,\gamma_t-2} + \zeta_1(4, 2) + 2\zeta_1(2, 2) + \zeta_1(2, 1) + 2[\zeta_1(4, 4) - \zeta_1(4, 3)]$$
$$= \xi_{p,\gamma_t} - \frac{4}{\sqrt{2}} + \sqrt{\frac{4}{6}} + 2\sqrt{\frac{2}{4}} + \sqrt{\frac{1}{3}} + 2\left[\sqrt{\frac{6}{8}} - \sqrt{\frac{5}{7}}\right]$$
$$= \xi_{p,\gamma_t} + 0.0214 > \xi_{p,\gamma_t}.$$

$\square$

Claim 8: Suppose that $d_{\alpha_1} = 1$, $d_{\alpha_2} = d_{\alpha_3} = d_{\alpha_4} = 2$, $d_{\alpha_5} = 3$, satisfying $\alpha_5 \in \mathscr{D}$. Then, $ABS(\mathscr{T}) > \xi_{p,\gamma_t}$ (see Figure 4).

Proof. For $d_{\theta_1} \leq 3$ and $d_{\alpha_6} \geq 2$, let $\mathscr{T}_9 = \mathscr{T} - \{\alpha_1, \alpha_2, \alpha_3, \alpha_4\}$. Then, as in Claim 7,

$$ABS(\mathscr{T}) = ABS(\mathscr{T}_9) - \zeta_1(d_{\alpha_6}, 2) + \zeta_1(d_{\alpha_6}, 3) + \zeta_1(3, 2) + 2\zeta_1(2, 2) + \zeta_1(2, 1)$$
$$+ \zeta_1(d_{\theta_1}, 3) - \zeta_1(d_{\theta_1}, 2)$$
$$\geq \xi_{p-4,\gamma_t-2} + \zeta_1(3, 2) - \zeta_1(2, 2) + \zeta_1(3, 2) + 2\zeta_1(2, 2) + \zeta_1(2, 1) + \zeta_1(3, 3)$$
$$- \zeta_1(3, 2)$$
$$= \xi_{p,\gamma_t} - \frac{4}{\sqrt{2}} + \sqrt{\frac{3}{5}} - \sqrt{\frac{2}{4}} + 2\sqrt{\frac{2}{4}} + \frac{1}{\sqrt{3}} + \sqrt{\frac{4}{6}} = \xi_{p,\gamma_t} + 0.0471 > \xi_{p,\gamma_t}.$$
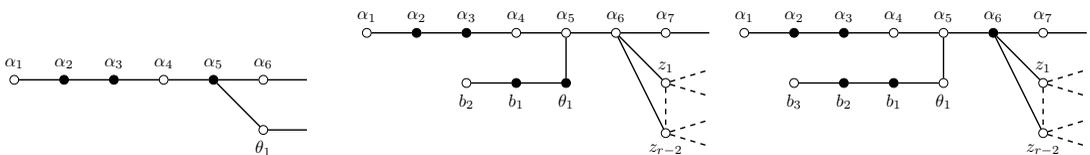
$\square$

Figure 4: Sample trees for Claims 8, 9 and 10, respectively.

Claim 9: Suppose that $b_2b_1\theta_1\alpha_5$ be a path attached to α_5 such that $d_{b_2} = 1, d_{b_1} = d_{\theta_1} = 2, d_{\alpha_5} = 3$ with $d_{\alpha_1} = 1, d_{\alpha_2} = d_{\alpha_3} = d_{\alpha_4} = 2, d_{\alpha_6} \geq 2$. If $d_{z_m} \leq 3, m \in \{1, \cdots, r-2\}$, then, $ABS(\mathscr{T}) > \xi_{p,\gamma_t}$ (see Figure 4).

Proof. Assume $\alpha_4, \alpha_5 \notin \mathscr{D}$. Let $\mathscr{T}_{10} = \mathscr{T} - \{\alpha_1, \alpha_2, \alpha_3, \alpha_4, \alpha_5, \theta_1, b_1, b_2\}$. Then,

$$
\begin{aligned}
ABS(\mathscr{T}) &= ABS(\mathscr{T}_{10}) + 2\zeta_1(2,1) - \zeta_1(d_{\alpha_7}, r-1) + \zeta_1(d_{\alpha_7}, r) + \zeta_1(r,3) + 2\zeta_1(3,2) \\
&\quad + 3\zeta_1(2,2) + \sum_{m=1}^{r-2} \left[\zeta_1(d_{z_m}, r) - \zeta_1(d_{z_m}, r-1) \right] \\
&> \xi_{p-8,\gamma_t-4} + \zeta_1(3,2) + 2\zeta_1(3,2) + 3\zeta_1(2,2) + 2\zeta_1(2,1) + \zeta_1(3,2) - \zeta_1(3,1) \\
&= \xi_{p,\gamma_t} - \frac{8}{\sqrt{2}} + 4\sqrt{\frac{3}{5}} + 2\sqrt{\frac{2}{4}} + 2\sqrt{\frac{1}{3}} \\
&= \xi_{p,\gamma_t} + 0.0104 > \xi_{p,\gamma_t}.
\end{aligned}
$$

$\square$

Claim 10: Suppose that, $b_3b_2b_1\theta_1\alpha_5$ be a path attached to α_5 such that $d_{b_3} = 1, d_{b_2} = d_{b_1} = d_{\theta_1} = 2, d_{\alpha_5} = 3$ with $d_{\alpha_1} = 1, d_{\alpha_2} = d_{\alpha_3} = d_{\alpha_4} = 2$. Then, $ABS(\mathscr{T}) > \xi_{p,\gamma_t}$ (see Figure 4).

Proof. Let $\alpha_5 \notin \mathscr{D}, \alpha_6 \in \mathscr{D}$. Take $\mathscr{T}_{11} = \mathscr{T} - \{\alpha_1, \alpha_2, \alpha_3, \alpha_4, \theta_1, b_1, b_2, b_3\}$.

$$
\begin{aligned}
ABS(\mathscr{T}) &= ABS(\mathscr{T}_{11}) - \zeta_1(r,1) + \zeta_1(r,3) + 2\zeta_1(3,2) + 4\zeta_1(2,2) + 2\zeta_1(2,1) \\
&\geq \xi_{p-8,\gamma_t-4} - \zeta_1(2,1) + \zeta_1(3,2) + 2\zeta_1(3,2) + 4\zeta_1(2,2) + 2\zeta_1(2,1) \\
&= \xi_{p,\gamma_t} - \frac{8}{\sqrt{2}} + 3\sqrt{\frac{3}{5}} + 4\sqrt{\frac{2}{4}} + \sqrt{\frac{1}{3}} \\
&= \xi_{p,\gamma_t} + 0.0727 > \xi_{p,\gamma_t}.
\end{aligned}
$$

$\square$

Let $d_{\alpha_7} = s, N(\alpha_7) = \{\alpha_6, \alpha_8, y_1, \ldots, y_{s-2}\}$ and $d_{\alpha_8} = i, N(\alpha_8) = \{\alpha_7, \alpha_9, x_1, \ldots, x_{i-2}\}$. As $ABS(P_5) > \xi_{5,3}, ABS(P_6) > \xi_{6,4}$ and $ABS(P_7) > \xi_{7,4}$, it follows from Claims 1−10 that $d \geq 7$, $d_{\alpha_2} = d_{\alpha_3} = d_{\alpha_4} = d_{\alpha_5} = 2, \alpha_2, \alpha_3, \alpha_6 \in \mathscr{D}$ and $\alpha_4, \alpha_5 \notin \mathscr{D}$. Furthermore, one can assume that every vertex $z \in N(\alpha_6) \setminus \{\alpha_5, \alpha_7\}$ satisfies $d_z \leq 2$.

Case A: Choose $d_{\alpha_6} = 2$.
Take $\mathscr{T}_{12} = \mathscr{T} - \{\alpha_1, \alpha_2, \alpha_3, \alpha_4\}$. Then,

$$
\begin{aligned}
ABS(\mathscr{T}) &= ABS(\mathscr{T}_{12}) + \zeta_1(2,2) + 3\zeta_1(2,2) + \zeta_1(2,1) - \zeta_1(2,1) \\
&\geq \xi_{p-4,\gamma_t-2} + 4\zeta_1(2,2) \\
&= \xi_{p,\gamma_t} - \frac{4}{\sqrt{2}} + 4\sqrt{\frac{2}{4}} = \xi_{p,\gamma_t},
\end{aligned}
$$

the equality being observed whenever $\mathscr{T}_{12} \in \mathscr{T}_{p-4,\gamma_t-2}$ which implies $\mathscr{T} \in \mathscr{G}_{p,\gamma_t}$.

Case B: Suppose $d_{\alpha_6} = 3$.
Case B.1: Take $d_{z_1} = 1$.

M. Manuel and A. Parthiban

Malaysian J. Math. Sci. 20(1): 21–42(2026) *21 - 42*

Case B.1.1: Assume $d_{\alpha_7} \leq 3$.

Take $\mathscr{T}_{13} = \mathscr{T} - \{\alpha_1, \alpha_2, \alpha_3, \alpha_4, \alpha_5\}$. Then,

$$
\begin{aligned}
ABS(\mathscr{T}) &= ABS(\mathscr{T}_{13}) - \zeta_1(d_{\alpha_7}, 2) + \zeta_1(d_{\alpha_7}, 3) - \zeta_1(2, 1) + \zeta_1(3, 1) + \zeta_1(3, 2) \\
&\quad + 3\zeta_1(2, 2) + \zeta_1(2, 1) \\
&\geq \xi_{p-5, \gamma_t - 2} + \zeta_1(3, 3) + \zeta_1(3, 2) + 3\zeta_1(2, 2) + \zeta_1(3, 1) - \zeta_1(3, 2) \\
&= \xi_{p, \gamma_t} - \left(\frac{1 + \sqrt{2}}{\sqrt{6}} + \frac{2\sqrt{3}}{\sqrt{5}} - \frac{5}{2\sqrt{2}} \right) + 3\sqrt{\frac{2}{4}} + \sqrt{\frac{2}{4}} + \sqrt{\frac{4}{6}} - \frac{4}{\sqrt{2}} \\
&= \xi_{p, \gamma_t} + 0.0495 > \xi_{p, \gamma_t}.
\end{aligned}
$$

Case B.1.2: Consider $d_{\alpha_7} \geq 4$.

Case B.1.2.1: Let $|N(\alpha_7) \cap \mathscr{D}| \geq 2$. Take $\mathscr{T}_{14} = \mathscr{T} - \{\alpha_1, \alpha_2, \alpha_3, \alpha_4, \alpha_5, \alpha_6, z_1\}$. Then,

$$
\begin{aligned}
ABS(\mathscr{T}) &= ABS(\mathscr{T}_{14}) - \zeta_1(d_{\alpha_8}, s - 1) + \zeta_1(d_{\alpha_8}, s) + \zeta_1(s, 3) + \zeta_1(3, 2) \\
&\quad + \zeta_1(3, 1) + 3\zeta_1(2, 2) + \zeta_1(2, 1) \\
&\quad + \sum_{m=1}^{s-2} \left[\zeta_1(d_{y_m}, s) - \zeta_1(d_{y_m}, s - 1) \right] \\
&> \xi_{p-7, \gamma_t - 3} + \zeta_1(4, 3) + \zeta_1(3, 2) + \zeta_1(3, 1) + 3\zeta_1(2, 2) + \zeta_1(2, 1) \\
&= \xi_{p, \gamma_t} - \left(\frac{1 + \sqrt{2}}{\sqrt{6}} + \frac{2\sqrt{3}}{\sqrt{5}} - \frac{5}{2\sqrt{2}} \right) - \frac{6}{\sqrt{2}} + \sqrt{\frac{5}{7}} + 3\sqrt{\frac{2}{4}} \\
&\quad + \sqrt{\frac{2}{4}} + \sqrt{\frac{3}{5}} + \sqrt{\frac{1}{3}} \\
&= \xi_{p, \gamma_t} + 0.0159 > \xi_{p, \gamma_t}.
\end{aligned}
$$

Case B.1.2.2: Let $N(\alpha_7) \cap \mathscr{D} = \{\alpha_6\}$.

Case B.1.2.2.a: If $d_{y_1} \geq 2$, by the claims proved above, there is a pendant path $\alpha_7 y_1 a_1 a_2 a_3 a_4$ attached to α_7 such that $d_{y_1} = d_{a_1} = d_{a_2} = d_{a_3} = 2, d_{a_4} = 1$. Since $d_{\alpha_7} \geq 4$, one can obtain $ABS(\mathscr{T}) > \xi_{p, \gamma_t}$ by considering the above cases.

Case B.1.2.2.b: For $d_{y_m} = 1, m \in \{1, 2, \ldots, s - 2\}$, take $\mathscr{T}_{15} = \mathscr{T} - \{y_1\}$. Then,

$$
\begin{aligned}
ABS(\mathscr{T}) &= ABS(\mathscr{T}_{15}) - \zeta_1(d_{\alpha_8}, s - 1) + \zeta_1(d_{\alpha_8}, s) - \zeta_1(s - 1, 3) + \zeta_1(s, 1) \\
&\quad + \zeta_1(s, 3) + (s - 3)[\zeta_1(s, 1) - \zeta_1(s - 1, 1)] \\
&> \xi_{p-1, \gamma_t} + \zeta_1(4, 3) - \zeta_1(3, 3) + \zeta_1(4, 1) \\
&= \xi_{p, \gamma_t} - \left(\frac{1 + \sqrt{2}}{\sqrt{6}} + \frac{2\sqrt{3}}{\sqrt{5}} - \frac{5}{2\sqrt{2}} \right) + \sqrt{\frac{5}{7}} - \sqrt{\frac{4}{6}} + \sqrt{\frac{3}{5}} \\
&= \xi_{p, \gamma_t} + 0.0362 > \xi_{p, \gamma_t}.
\end{aligned}
$$

Case B.2: Assume $d_{z_1} = 2$.

From the claims proved above, there is a pendant path $\alpha_6 z_1 c_1 c_2 c_3 c_4$ attached to α_6 with $d_{c_1} = d_{c_2} = d_{c_3} = 2, d_{c_4} = 1$.

Case B.2.1: Suppose $d_{\alpha_7} = 2$.

Take $\mathscr{T}_{16} = \mathscr{T} - \{\alpha_1, \alpha_2, \alpha_3, \alpha_4, \alpha_5\}$. Then

$$
\begin{aligned}
ABS(\mathscr{T}) &= ABS(\mathscr{T}_{16}) - \zeta_1(d_{\alpha_7}, 2) + \zeta_1(d_{\alpha_7}, 3) - \zeta_1(2, 2) + \zeta_1(3, 2) + \zeta_1(3, 2) \\
&\quad + 3\zeta_1(2, 2) + \zeta_1(2, 1) \\
&\geq \xi_{p-5, \gamma_t - 2} + 3\zeta_1(3, 2) + \zeta_1(2, 2) + \zeta_1(2, 1) \\
&= \xi_{p, \gamma_t} - \left(\frac{1 + \sqrt{2}}{\sqrt{6}} + \frac{2\sqrt{3}}{\sqrt{5}} - \frac{5}{2\sqrt{2}} \right) - \frac{4}{\sqrt{2}} + 3\sqrt{\frac{3}{5}} + \sqrt{\frac{2}{4}} + \sqrt{\frac{1}{3}} \\
&= \xi_{p, \gamma_t} + 0.0128 > \xi_{p, \gamma_t}.
\end{aligned}
$$

Case B.2.2: Choose $d_{\alpha_7} \geq 3$.

Case B.2.2.1: Let $|N(\alpha_7) \cap \mathscr{D}| \geq 2$.

By considering the above claims and cases, let $d_{y_m} \leq 3$, $m \in \{1, 2, \ldots, s - 2\}$ and $d_{\alpha_8} \geq 2$.

Take $\mathscr{T}_{17} = \mathscr{T} - \{\alpha_1, \alpha_2, \alpha_3, \alpha_4, \alpha_5, \alpha_6, z_1, c_1, c_2, c_3, c_4\}$. Then,

$$
\begin{aligned}
ABS(\mathscr{T}) &= ABS(\mathscr{T}_{17}) - \zeta_1(d_{\alpha_8}, s - 1) + \zeta_1(d_{\alpha_8}, s) + \zeta_1(s, 3) + 2\zeta_1(3, 2) \\
&\quad + 6\zeta_1(2, 2) + 2\zeta_1(2, 1) \\
&\quad + \sum_{m=1}^{s-2} [\zeta_1(d_{y_m}, s) - \zeta_1(d_{y_m}, s - 1)] \\
&\geq \xi_{p-11, \gamma_t - 5} - \zeta_1(3, 2) + \zeta_1(3, 3) + \zeta_1(3, 3) + 2\zeta_1(3, 2) + 6\zeta_1(2, 2) \\
&\quad + 2\zeta_1(2, 1) + \zeta_1(3, 2) - \zeta_1(2, 2) \\
&= \xi_{p, \gamma_t} - \left(\frac{1 + \sqrt{2}}{\sqrt{6}} + \frac{2\sqrt{3}}{\sqrt{5}} - \frac{5}{2\sqrt{2}} \right) - \frac{10}{\sqrt{2}} + 2\sqrt{\frac{4}{6}} + 2\sqrt{\frac{3}{5}} \\
&\quad + 5\sqrt{\frac{2}{4}} + 2\sqrt{\frac{1}{3}} \\
&= \xi_{p, \gamma_t} + 0.0343 > \xi_{p, \gamma_t}.
\end{aligned}
$$

Case B.2.2.2: Let $N(\alpha_7) \cap \mathscr{D} = \{\alpha_6\}$.

From the claims, suppose $d_{y_m} \leq 2$, $m \in \{1, 2, \ldots, s - 2\}$.

Case B.2.2.2.a: Fix $d_{y_1} = 1$.

Case B.2.2.2.a.1: While $d_{\alpha_7} \geq 4$, take $\mathscr{T}_{18} = \mathscr{T} - \{y_1\}$. Then,

$$
\begin{aligned}
ABS(\mathscr{T}) &= ABS(\mathscr{T}_{18}) + \zeta_1(d_{\alpha_8}, s) - \zeta_1(d_{\alpha_8}, s - 1) - \zeta_1(s - 1, 3) + \zeta_1(s, 3) \\
&\quad + \zeta_1(s, 1) + \sum_{m=1}^{s-2} [\zeta_1(d_{y_m}, s) - \zeta_1(d_{y_m}, s - 1)] \\
&> \xi_{p-1, \gamma_t} + \zeta_1(4, 1) + \zeta_1(4, 3) - \zeta_1(3, 3) \\
&= \xi_{p, \gamma_t} - \left(\frac{1 + \sqrt{2}}{\sqrt{6}} + \frac{2\sqrt{3}}{\sqrt{5}} - \frac{5}{2\sqrt{2}} \right) + \sqrt{\frac{3}{5}} + \sqrt{\frac{5}{7}} - \sqrt{\frac{4}{6}} \\
&= \xi_{p, \gamma_t} + 0.0362 > \xi_{p, \gamma_t}.
\end{aligned}
$$

Case B.2.2.2.a.2: Let $d_{\alpha_7} = 3$.

Case B.2.2.2.a.2.1: While $d_{\alpha_8} \leq 3$, take $\mathscr{T}_{19} = \mathscr{T} - \{y_1, z_1, c_1, c_2, c_3, c_4\}$. Then,

$$
\begin{aligned}
ABS(\mathscr{T}) &= ABS(\mathscr{T}_{19}) - \zeta_1(d_{\alpha_8}, 2) + \zeta_1(d_{\alpha_8}, 3) - \zeta_1(2,2) + \zeta_1(3,2) \\
&\quad - \zeta_1(2,2) + \zeta_1(3,3) + \zeta_1(3,1) + \zeta_1(3,2) + 3\zeta_1(2,2) + \zeta_1(2,1) \\
&\geq \xi_{p-6, \gamma_t - 2} + 2\zeta_1(3,3) + \zeta_1(3,2) + \zeta_1(2,2) + \zeta_1(3,1) + \zeta_1(2,1) \\
&= \xi_{p,\gamma_t} - 2\left(\frac{1+\sqrt{2}}{\sqrt{6}} + \frac{2\sqrt{3}}{\sqrt{5}} - \frac{5}{2\sqrt{2}} \right) - \frac{4}{\sqrt{2}} + 2\sqrt{\frac{4}{6}} + \sqrt{\frac{3}{5}} \\
&\quad + \sqrt{\frac{2}{4}} + \sqrt{\frac{2}{4}} + \sqrt{\frac{1}{3}} \\
&= \xi_{p,\gamma_t} + 0.0367 > \xi_{p,\gamma_t}.
\end{aligned}
$$

Case B.2.2.2.a.2.2: Let $d_{\alpha_8} \geq 4$.

Case B.2.2.2.a.2.2.1: If $|N(\alpha_8) \cap \mathscr{D}| \geq 2$, take $\mathscr{T}_{20}$ and $\mathscr{T}_{21}$ as sub-trees of $\mathscr{T} - \alpha_7 \alpha_8$ containing α_7 and α_8, respectively, then

$$
\begin{aligned}
ABS(\mathscr{T}) &= ABS(\mathscr{T}_{20}) + ABS(\mathscr{T}_{21}) - \zeta_1(3,2) + \zeta_1(3,3) - \zeta_1(2,1) \\
&\quad + \zeta_1(3,1) + \zeta_1(i,3) - \zeta_1(d_{\alpha_9}, i-1) + \zeta_1(d_{\alpha_9}, i) \\
&\quad + \sum_{m=1}^{i-2} \left[\zeta_1(d_{x_m}, i) - \zeta_1(d_{x_m}, i-1) \right] \\
&\geq \xi_{p,\gamma_t} + \frac{2}{\sqrt{3}} - \frac{3}{\sqrt{2}} - \zeta_1(2,1) - \zeta_1(3,2) + \zeta_1(4,3) + \zeta_1(3,1) \\
&\quad + \zeta_1(3,3) \\
&= \xi_{p,\gamma_t} + \frac{2}{\sqrt{3}} - \frac{3}{\sqrt{2}} + \sqrt{\frac{5}{7}} + \sqrt{\frac{2}{4}} + \sqrt{\frac{4}{6}} - \sqrt{\frac{1}{3}} - \sqrt{\frac{3}{5}} \\
&= \xi_{p,\gamma_t} + 0.0502 > \xi_{p,\gamma_t}.
\end{aligned}
$$

Case B.2.2.2.a.2.2.2: Let $N(\alpha_8) \cap \mathscr{D} = \{\alpha_7\}$. Any path from α_8 to a pendant vertex through $\alpha_8 x_m, m \in \{1, 2, \ldots, i-2\}$ has length 4. From the claims, $ABS(\mathscr{T}) > \xi_{p,\gamma_t}$ can be obtained.

Case B.2.2.2.b: Suppose that $d_{y_m} = 2, m \in \{1, 2, \ldots, s-2\}$. Any path from α_7 to a pendant vertex through $\alpha_7 y_m, m \in \{1, 2, \ldots, s-2\}$ has length 5. From the above cases and $d_{\alpha_7} \geq 3$ implies $d_{\alpha_7} = 3$.

Hence, there is a pendant path $\alpha_7 y_1 a_1 a_2 a_3 a_4$ attached to α_7 on 6 vertices such that $d_{y_1} = d_{a_1} = d_{a_2} = d_{a_3} = 2$ and $d_{a_4} = 1$.

Case B.2.2.2.b.1: Suppose $d_{\alpha_8} = 2$.

Take $\mathscr{T}_{22} = \mathscr{T} - \{z_1, c_1, c_2, c_3, c_4, y_1, a_1, a_2, a_3, a_4\}$. Then,

$$
\begin{aligned}
ABS(\mathscr{T}) &= ABS(\mathscr{T}_{22}) - \zeta_1(2,2) + \zeta_1(3,3) - 2\zeta_1(2,2) + 2\zeta_1(3,2) \\
&\quad + 6\zeta_1(2,2) + 2\zeta_1(3,3) + 2\zeta_1(2,1) \\
&\geq \xi_{p-10, \gamma_t - 4} + \zeta_1(3,3) + 4\zeta_1(3,2) + 3\zeta_1(2,2) + 2\zeta_1(2,1) \\
&= \xi_{p,\gamma_t} - 2\left(\frac{1+\sqrt{2}}{\sqrt{6}} + \frac{2\sqrt{3}}{\sqrt{5}} - \frac{5}{2\sqrt{2}} \right) - \frac{8}{\sqrt{2}} + \sqrt{\frac{4}{6}} + 4\sqrt{\frac{3}{5}} \\
&\quad + 3\sqrt{\frac{2}{4}} + 2\sqrt{\frac{1}{3}} \\
&= \xi_{p,\gamma_t},
\end{aligned}
$$

with the equality is intact when $\mathscr{T}_{22} \in \mathscr{T}_{p-10, \gamma_t - 4}$ implies $\mathscr{T} \in \mathscr{G}_{p,\gamma_t}$.

Case B.2.2.2.b.2: Consider $d_{\alpha_8} \geq 3$.

Case B.2.2.2.b.2.1: If $d_{x_m} \leq 3$; $m \in \{1, \ldots, i-2\}$ and $|N(\alpha_8) \cap \mathscr{D}| \geq 2$, take $\mathscr{T}_{23}$ and $\mathscr{T}_{24}$ as sub-trees of $\mathscr{T} - \alpha_7\alpha_8$ containing α_7 and α_8, respectively, then,

$$
\begin{aligned}
ABS(\mathscr{T}) &= ABS(\mathscr{T}_{23}) + ABS(\mathscr{T}_{24}) - \zeta_1(2,2) - \zeta_1(3,2) + \zeta_1(3,3) \\
&\quad + \zeta_1(3,2) + \zeta_1(i,3) - \zeta_1(d_{\alpha_9}, i-1) + \zeta_1(d_{\alpha_9}, i) \\
&\quad + \sum_{m=1}^{i-2} [\zeta_1(d_{x_m}, i) - \zeta_1(d_{x_m}, i-1)] \\
&\geq ABS(\mathscr{T}_{23}) + ABS(\mathscr{T}_{24}) + \zeta_1(3,3) + \zeta_1(3,2) - \zeta_1(2,2) \\
&\quad + \zeta_1(3,3) - \zeta_1(3,2) + \zeta_1(3,3) - \zeta_1(3,2) \\
&= 10\zeta_1(2,2) + 3\zeta_1(3,2) + 3\zeta_1(2,1) + ABS(\mathscr{T}_{24}) + 3\zeta_1(3,3) \\
&\quad - \zeta_1(2,2) - \zeta_1(3,2) \\
&\geq \xi_{p-17,\gamma_t-8} + 2\zeta_1(3,2) + 3\zeta_1(2,1) + 9\zeta_1(2,2) + 3\zeta_1(3,3) \\
&= \xi_{p,\gamma_t} - \left(\frac{1+\sqrt{2}}{\sqrt{6}} + \frac{2\sqrt{3}}{\sqrt{5}} - \frac{5}{2\sqrt{2}} \right) - \frac{16}{\sqrt{2}} + 2\sqrt{\frac{3}{5}} + 3\sqrt{\frac{1}{3}} \\
&\quad + 9\sqrt{\frac{2}{4}} + 3\sqrt{\frac{4}{6}} \\
&= \xi_{p,\gamma_t} + 0.0139 > \xi_{p,\gamma_t}.
\end{aligned}
$$

Case B.2.2.2.b.2.2: Let $N(\alpha_8) \cap \mathscr{D} = \{\alpha_7\}$.

Any path from α_8 to a pendant vertex through $\alpha_8 x_m$, $m \in \{1, 2, \ldots, i-2\}$ has length 4. From the claims, $ABS(\mathscr{T}) > \xi_{p,\gamma_t}$ can be obtained.

Case C: Let $d_{\alpha_6} \geq 4$.

While $d_{z_m} \leq 2$, $m \in \{1, \ldots, r-2\}$, take $\mathscr{T}_{25} = \mathscr{T} - \{\alpha_1, \alpha_2, \alpha_3, \alpha_4, \alpha_5\}$.

$$
\begin{aligned}
ABS(\mathscr{T}) &= ABS(\mathscr{T}_{25}) - \zeta_1(d_{\alpha_7}, r-1) + \zeta_1(d_{\alpha_7}, r) + \zeta_1(r,2) + 3\zeta_1(2,2) + \zeta_1(2,1) \\
&\quad + \sum_{m=1}^{r-2} [\zeta_1(d_{z_m}, r) - \zeta_1(d_{z_m}, r-1)] \\
&> \xi_{p-5,\gamma_t-2} + \zeta_1(4,2) + 3\zeta_1(2,2) + \zeta_1(2,1) + 2[\zeta_1(4,2) - \zeta_1(3,2)] \\
&= \xi_{p,\gamma_t} - \left(\frac{1+\sqrt{2}}{\sqrt{6}} + \frac{2\sqrt{3}}{\sqrt{5}} - \frac{5}{2\sqrt{2}} \right) - \frac{4}{\sqrt{2}} + 3\sqrt{\frac{4}{6}} + 3\sqrt{\frac{2}{4}} + \sqrt{\frac{1}{3}} - 2\sqrt{\frac{3}{5}} \\
&= \xi_{p,\gamma_t} + 0.0035 > \xi_{p,\gamma_t}.
\end{aligned}
$$

$\hspace{14cm}\square$

4 Applications to the QSPR Studies of Carboxylic Acids

Carboxylic acids are a class of organic compounds characterized by the presence of a carboxyl functional group ($-COOH$), which significantly influences their chemical behavior and physical properties. A set of 17 carboxylic acids was selected to examine the significance of the derived lower bound through structural and quantitative analysis. The chemical graphs corresponding to these compounds were generated from their molecular structures (see Figure 5), where atoms

are represented as vertices and bonds as edges. In this graph-theoretical representation, distinctions between single and double bonds were omitted and hydrogen atoms were excluded from the vertex set [24]. The chemical structure diagrams were sourced from the PubChem database [19].
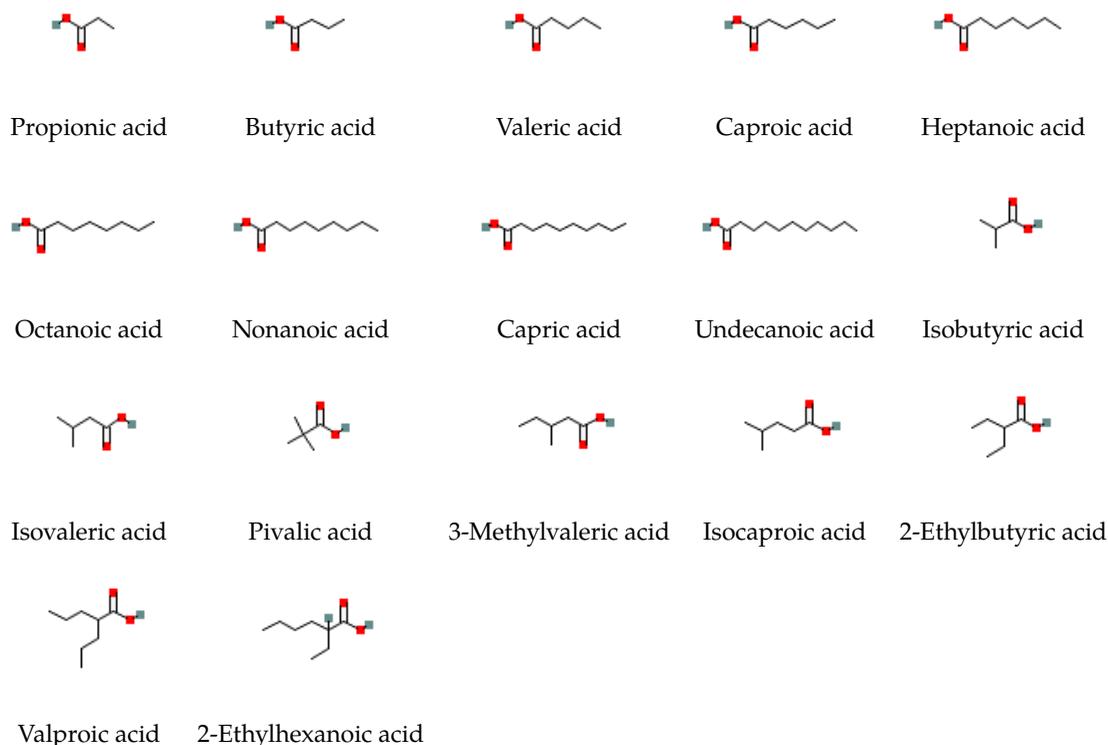

Figure 5: Chemical structures of the selected carboxylic acids.

Quantitative Structure-Property Relationship (QSPR) analysis is a powerful computational method that establishes correlations between molecular structure and experimentally measured physicochemical properties using mathematical descriptors. This approach facilitates the interpretation and prediction of chemical properties across structurally diverse compounds. In this study, QSPR analysis was applied to evaluate the selected carboxylic acids with respect to various physicochemical properties, including boiling point (BP), logarithm of the partition coefficient ($\log P$) between octanol and water, density (ρ), measure of cytotoxicity ($\log(1/IGC_{50})$) (based on the 50% inhibitory growth concentration), molecular weight (MW), polarizability (α), enthalpy of vaporization (EV), flash point (FP), index of refraction (RI) and molar volume (MV). The experimental values for these properties were obtained from PubChem [19], ChemSpider [21] and other literature sources [18], as summarized in Table 2.

Table 2: Physicochemical properties of the selected carboxylic acids.

Name	BP (°C)	log P	ρ (g/cm^3)	log(1/IGC$_{50}$)	MW (g/mol)	α (Å^3)	EV (kJ/mol)	FP (°C)	RI	MV (cm^3/mol)
Propionic acid	141.1	0.33	0.99	-0.5123	74.08	6.9	40.1	51.7	1.397	72.7
Butyric acid	163.7	0.79	0.96	-0.572	88.11	8.8	42.4	76.7	1.411	89.2
Valeric acid	185.4	1.39	0.94	-0.2674	102.13	10.6	44.6	88.9	1.421	105.7
Caproic acid	205.8	1.92	0.93	-0.2083	116.16	12.5	46.6	104.4	1.428	122.2
Heptanoic acid	222.2	2.42	0.90	-0.1126	130.18	14.3	48.5	99.2	1.433	138.7
Octanoic acid	239.0	3.05	0.91	0.0807	144.21	16.1	50.3	107.4	1.437	155.2
Nonanoic acid	254.5	3.42	0.90	0.3509	158.24	18.0	52.0	100.0	1.441	171.7
Capric acid	268.7	4.09	0.89	0.5063	172.26	19.8	53.6	121.8	1.443	188.2
Undecanoic acid	227.9	4.42	0.89	0.8983	186.29	21.6	55.2	128.2	1.446	204.7
Isobutyric acid	154.4	0.94	0.95	-0.3334	88.11	8.8	43.2	55.6	1.408	89.6
Isovaleric acid	176.5	1.16	0.93	-0.3415	102.13	10.6	45.4	70.6	1.418	106.1
Pivalic acid	163.8	1.48	0.91	-0.2543	102.13	10.6	44.4	68.3	1.420	105.7
3-Methylvaleric acid	196.0	1.66	0.93	-0.2331	116.16	12.4	48.0	85.0	1.425	122.6
Isocaproic acid	199.0	1.66	0.92	-0.2724	116.16	12.4	48.2	97.2	1.425	122.6
2-Ethylbutyric acid	99.0	1.68	0.92	-0.1523	116.16	12.4	47.6	87.8	1.425	122.6
Valproic acid	220.0	2.75	0.91	0.0258	144.21	16.1	50.3	111.1	1.435	155.6
2-Ethylhexanoic acid	228.0	2.64	0.90	0.0756	144.21	16.1	51.2	116.6	1.435	155.6

4.1 Linear regression models using ξ_{p,γ_t}

The QSPR analysis for the selected carboxylic acids was conducted using the ξ_{p,γ_t} values, derived from their molecular graphs. A linear regression model was employed at a 95% confidence level, where statistical significance is established only if the associated p-values (probability) are less than 0.05. The analysis is based on the linear regression equation $Y = C_0 + C_1(\xi_{p,\gamma_t})$, where Y denotes the target physicochemical property, C_0 is the regression intercept and C_1 represents the regression coefficient associated with ξ_{p,γ_t}. The computed values of ξ_{p,γ_t} for the 17 carboxylic acids, along with their total domination numbers extracted from the corresponding chemical graphs, are presented in Table 3.

Table 3: Computed ξ_{p,γ_t} values of the carboxylic acids.

Sl No.	Name	Chem. formula	p	γ_t	ξ_{p,γ_t}
1	Propionic acid	$C_3H_6O_2$	5	2	2.6288
2	Butyric acid	$C_4H_8O_2$	6	3	3.2760
3	Valeric acid	$C_5H_{10}O_2$	7	4	3.9233
4	Caproic acid	$C_6H_{12}O_2$	8	4	4.6903
5	Heptanoic acid	$C_7H_{14}O_2$	9	4	5.4573
6	Octanoic acid	$C_8H_{16}O_2$	10	5	6.1045
7	Nonanoic acid	$C_9H_{18}O_2$	11	6	6.7517
8	Capric acid	$C_{10}H_{20}O_2$	12	6	7.5187
9	Undecanoic acid	$C_{11}H_{22}O_2$	13	6	8.2857
10	Isobutyric acid	$C_4H_8O_2$	6	2	3.3958
11	Isovaleric acid	$C_5H_{10}O_2$	7	3	4.0430
12	Pivalic acid	$C_5H_{10}O_2$	7	2	4.1628
13	3-Methylvaleric acid	$C_6H_{12}O_2$	8	4	4.6903
14	Isocaproic acid	$C_6H_{12}O_2$	8	4	4.6903
15	2-Ethylbutyric acid	$C_6H_{12}O_2$	8	4	4.6903
16	Valproic acid	$C_8H_{16}O_2$	10	6	5.9847
17	2-Ethylhexanoic acid	$C_8H_{16}O_2$	10	5	6.1045

The results of the regression analysis are summarized in Table 4, where r denotes the correlation coefficient, R^2 s the coefficient of determination, SE represents the standard error of the estimate and p_F is the $p-$value (probability) associated with the Fisher's $F-$statistic used to assess the overall significance of the model.

Table 4: Linear regression analysis of the physicochemical properties of the selected carboxylic acids.

	r	R^2	SE	$F-$statistic	p_F	C_0	C_1
BP	0.7808	0.6096	28.2590	23.4211	2.16E-04	84.0710	22.1741
log P	0.9937	0.9874	0.1339	1177.1173	1.14E-15	-1.6790	0.7447
ρ	0.8792	0.7730	0.0131	51.0770	3.35E-06	0.9994	-0.0152
$\log(1/IGC_{50})$	0.9634	0.9281	0.1040	193.6490	5.57E-10	-1.2706	0.2347
MW	0.9991	0.9982	1.3617	8285.8780	5.42E-22	21.4479	20.0968
α	0.9991	0.9981	0.1808	8058.8872	6.68E-22	0.0370	2.6317
EV	0.9824	0.9651	0.7922	414.2391	2.45E-12	34.4550	2.6142
FP	0.8999	0.8098	10.0586	63.8607	8.73E-07	26.1463	13.0329
RI	0.9568	0.9154	0.0040	162.2671	1.90E-09	1.3849	0.0082
MV	0.9990	0.9981	1.6487	7807.6706	8.46E-22	11.0533	23.6209

Accordingly, the linear regression models corresponding to each physicochemical property are listed below (refer (1)),

$$
\begin{aligned}
BP &= 84.0710 + 22.1741(\xi_{p,\gamma_t}), \\
\log P &= -1.6790 + 0.7447(\xi_{p,\gamma_t}), \\
\rho &= 0.9994 - 0.0152(\xi_{p,\gamma_t}), \\
\log(1/\text{IGC}_{50}) &= -1.2706 + 0.2347(\xi_{p,\gamma_t}), \\
MW &= 21.4479 + 20.0968(\xi_{p,\gamma_t}), \\
\alpha &= 0.0370 + 2.6317(\xi_{p,\gamma_t}), \\
EV &= 34.4550 + 2.6142(\xi_{p,\gamma_t}), \\
FP &= 26.1463 + 13.0329(\xi_{p,\gamma_t}), \\
RI &= 1.3849 + 0.0082(\xi_{p,\gamma_t}), \\
MV &= 11.0533 + 23.6209(\xi_{p,\gamma_t}),
\end{aligned}
\tag{1}
$$

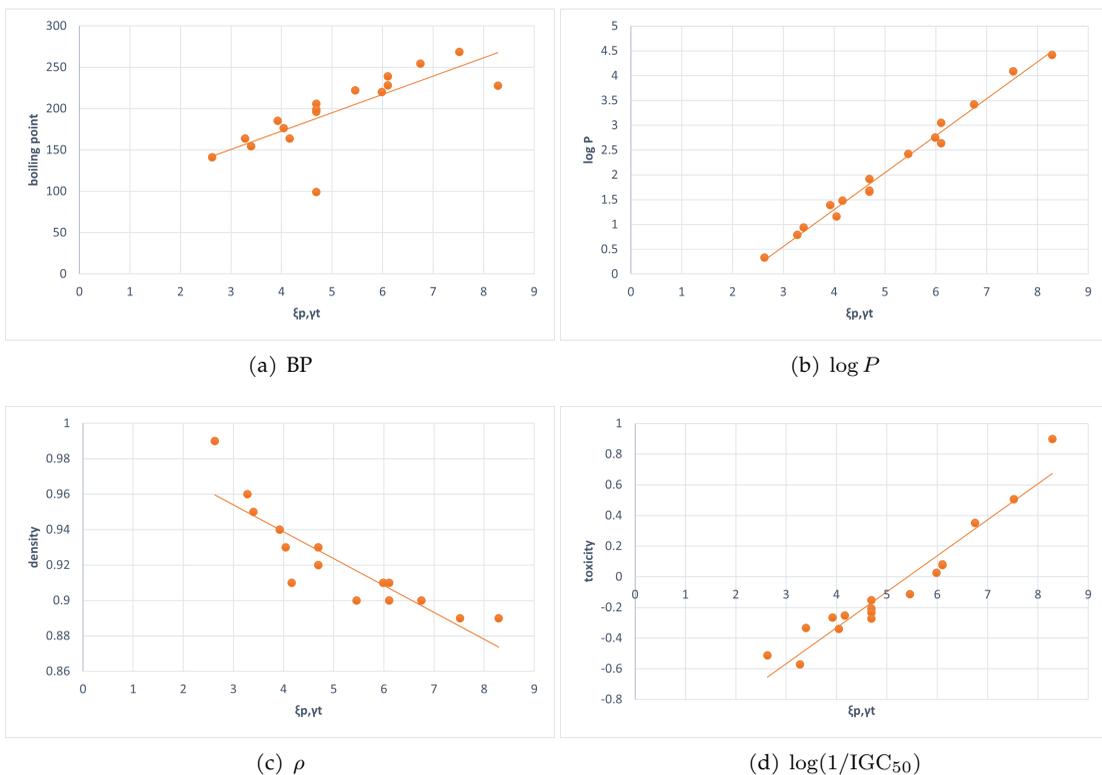while the associated linear regression curve plots are displayed in Figure 6.

(a) BP

(b) $\log P$

(c) ρ

(d) $\log(1/\text{IGC}_{50})$

Figure 6: Linear regression plots for the physicochemical properties of selected carboxylic acids, (a)–(d).

M. Manuel and A. Parthiban

Malaysian J. Math. Sci. 20(1): 21–42(2026) 21 - 42

(e) MW

(f) α

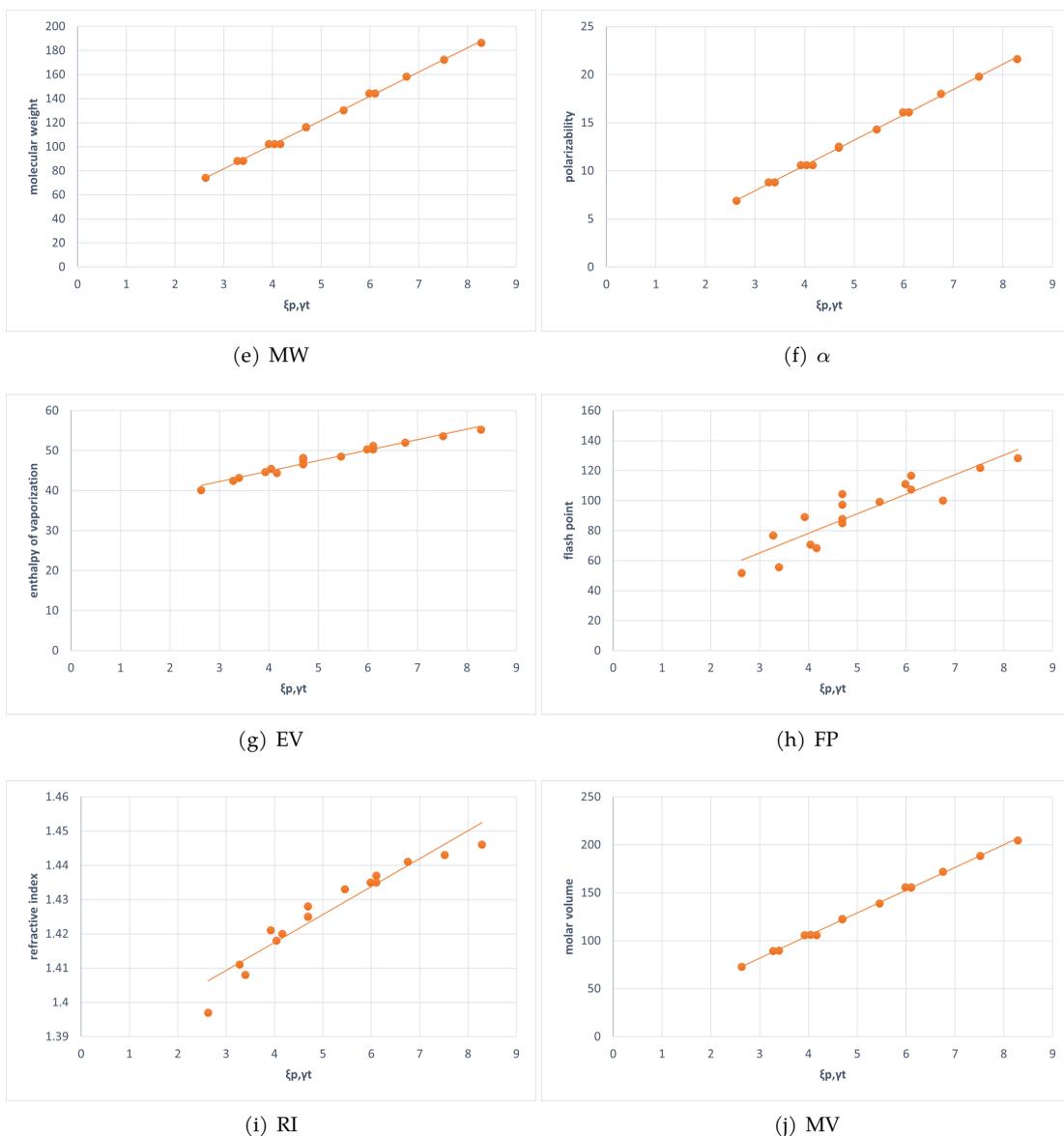(g) EV

(h) FP

(i) RI

(j) MV

Figure 6: (Continued) Linear regression plots for the physicochemical properties of selected carboxylic acids, (e)–(j).

4.2 Comparison of ABS with its variations

As mentioned in the introduction, the ABS index is a deviation of the ABC, SCI and R indices. Therefore, it is of interest to compare the performance of these indices in analyzing the physicochemical properties of the selected compounds. The computation of the topological indices was performed using the edge partition technique and the degree counting method, based on their respective definitions. The resulting values are summarized in Table 5.

Table 5: Computed values of selected topological indices for carboxylic acids.

Sl No.	Name	ABS	ABC	SCI	R
1	Propionic acid	2.7662	3.0472	2.0246	2.2701
2	Butyric acid	3.4733	3.7543	2.5246	2.7701
3	Valeric acid	4.1804	4.4614	3.0246	3.2701
4	Caproic acid	4.8875	5.1685	3.5246	3.7701
5	Heptanoic acid	5.5946	5.8756	4.0246	4.2701
6	Octanoic acid	6.3017	6.5827	4.5246	4.7701
7	Nonanoic acid	7.0088	7.2898	5.0246	5.2701
8	Capric acid	7.7159	7.9969	5.5246	5.7701
9	Undecanoic acid	8.4230	8.7041	6.0246	6.2701
10	Isobutyric acid	3.6449	3.9327	2.4082	2.6427
11	Isovaleric acid	4.3776	4.6812	2.8944	3.1259
12	Pivalic acid	4.5832	4.8766	2.7196	2.9434
13	3-Methylvaleric acid	5.0225	5.2779	3.419	3.6639
14	Isocaproic acid	5.0847	5.3873	3.3944	3.6259
15	2-Ethylbutyric acid	4.9346	5.1281	3.4574	3.7187
16	Valproic acid	6.3488	6.5423	4.4574	4.7187
17	2-Ethylhexanoic acid	6.3488	6.5423	4.4574	4.7187

The analysis is conducted on the same set of carboxylic acids and the correlation coefficients between each topological index and the specified physicochemical properties are presented in Table 6. The highest r values for each property are highlighted.

Table 6: Correlation coefficient (r) values of selected topological indices.

	BP	log P	ρ	$\log(1/\text{IGC}_{50})$	MW	α	EV	FP	RI	MV
ABS	0.7803	0.9897	**-0.8938**	0.9570	**0.9976**	0.9975	**0.9862**	0.8972	**0.9614**	**0.9977**
ABC	0.7864	0.9907	-0.8929	**0.9586**	0.9970	0.9969	0.9844	0.8938	0.9603	0.9971
SCI	**0.7917**	**0.9916**	-0.8478	0.9553	**0.9976**	**0.9978**	0.9780	0.9163	0.9547	0.9975
R	0.7899	0.9909	-0.8463	0.9543	0.9973	0.9974	0.9778	**0.9174**	0.9544	0.9972

4.3 Discussion

Based on Table 4, listed below are the observations from the linear regression analysis of the selected physicochemical properties of carboxylic acids using ξ_{p,γ_t},

1. The bound ξ_{p,γ_t} demonstrates excellent predictive capability for most physicochemical properties, especially molecular weight, polarizability, molar volume and $\log$ P, all showing near-perfect fits ($r = 0.99$). These properties, along with enthalpy of vaporization and toxicity, exhibit low standard errors and high $F-$statistic, indicating robust model performance.

2. FP ($r = 0.8999$) and RI ($r = 0.9568$) show good, albeit slightly lower, correlations compared to the highly correlated properties.

M. Manuel and A. Parthiban

Malaysian J. Math. Sci. 20(1): 21–42(2026) 21 - 42

3. The linear model appears less reliable for boiling point ($r = 0.7808$) and density ($r = 0.8792$), where the proportion of explained variance is comparatively lower.

4. Nevertheless, all models show statistical significance ($p_F < 0.05$), supporting the validity of the observed associations.

Based on the comparison of various topological indices for the selected carboxylic acid structures in Table 6, the following observations can be made;

1. The ABS index demonstrates consistently strong performance across most physicochemical properties, particularly for density, molecular weight, enthalpy of vaporization, refractive index and molar volume.

2. The SCI index performs slightly better for $\log$ P, polarizability, molecular weight and boiling point, while the ABC index shows marginally higher correlation for toxicity. The R index leads slightly in predicting flash point.

3. Overall, the differences in correlation values among the indices are minimal, suggesting that all four topological descriptors possess comparable predictive capabilities.

5   Conclusions

In this paper, we established a new lower bound for the atom-bond sum-connectivity (ABS) index of trees, formulated in terms of the total domination number and graph order. Additionally, we characterized the extremal trees that attain this bound, offering structural insights into the configurations that optimize this topological index under domination constraints. These theoretical findings deepen our understanding of the interplay between structural graph parameters and topological descriptors. While rooted in mathematical theory, the results hold practical relevance across domains where tree-like structures naturally arise. The applications proposed in this study span a range of fields, including chemical graph theory [4], network design (e.g., edge networks [29] and logical networks [26]), graph neural networks [30], physics-informed neural networks [15], structural analysis of computer networks [17] and emerging areas within deep learning [27]. By bridging discrete mathematics with practical applications, this work underscores the relevance of topological indices in both theoretical and applied contexts.

Conflicts of Interest The authors declare no conflict of interest.

References

[1] H. A. Ahangar & M. Khaibari (2017). Graphs with large Roman domination number. *Malaysian Journal of Mathematical Sciences*, 11(1), 71–81.

[2] A. A. S. Ahmad Jamri, F. Movahedi, R. Hasni, R. Gobithaasan & M. H. Akhbari (2022). Minimum Randić index of trees with fixed total domination number. *Mathematics*, 10(20), Article ID: 3729. https://doi.org/10.3390/math10203729.

[3] A. Ali, B. Furtula, I. Redžepović & I. Gutman (2022). Atom-bond sum-connectivity index. *Journal of Mathematical Chemistry*, *60*(10), 2081–2093. https://doi.org/10.1007/s10910-022-01403-1.

[4] A. Ali, I. Gutman & I. Redžepović (2023). Atom-bond sum-connectivity index of unicyclic graphs and some applications. *Electronic Journal of Mathematics*, *5*, 1–7. https://doi.org/10.47443/ejm.2022.039.

[5] S. Bermudo (2023). Upper bound for the geometric-arithmetic index of trees with given domination number. *Discrete Mathematics*, *346*(1), Article ID: 113172. https://doi.org/10.1016/j.disc.2022.113172.

[6] S. Bermudo, R. Hasni, F. Movahedi & J. E. Nápoles (2024). The Geometric–Arithmetic index of trees with a given total domination number. *Discrete Applied Mathematics*, *345*, 99–113. https://doi.org/10.1016/j.dam.2023.11.024.

[7] S. Bermudo, J. E. Nápoles & J. Rada (2020). Extremal trees for the Randić index with given domination number. *Applied Mathematics and Computation*, *375*, Article ID: 125122. https://doi.org/10.1016/j.amc.2020.125122.

[8] B. Borovićanin & B. Furtula (2016). On extremal Zagreb indices of trees with given domination number. *Applied Mathematics and Computation*, *279*, 208–218. https://doi.org/10.1016/j.amc.2016.01.017.

[9] E. J. Cockayne, R. M. Dawes & S. T. Hedetniemi (1980). Total domination in graphs. *Networks*, *10*(3), 211–219. https://doi.org/10.1002/net.3230100304.

[10] K. C. Das, I. Gutman & B. Furtula (2011). On atom-bond connectivity index. *Chemical Physics Letters*, *511*(4), 452–454. https://doi.org/10.1016/j.cplett.2011.06.049.

[11] Z. Du, B. Zhou & N. Trinajstić (2011). On the general sum-connectivity index of trees. *Applied Mathematics Letters*, *24*(3), 402–405. https://doi.org/10.1016/j.aml.2010.10.038.

[12] R. Hasni, D. A. Mojdeh & S. A. Bakar (2024). Domination (totally) dot-critical of Harary graphs. *Malaysian Journal of Mathematical Sciences*, *18*(1), 1–7. https://doi.org/10.47836/mjms.18.1.01.

[13] R. Hasni, A. A. S. Ahmad Jamri, N. E. Arif & F. N. Harun (2021). The Randić index of trees with given total domination number. *Iranian Journal of Mathematical Chemistry*, *12*(4), 225–237. https://doi.org/10.22052/ijmc.2021.243170.1591.

[14] T. W. Haynes, S. T. Hedetniemi & M. A. Henning (2020). *Topics in Domination in Graphs* volume 64. Springer, Cham.

[15] Y. He, E. Zio, Z. Yang, Q. Xiang, L. Fan, Q. He, S. Peng, Z. Zhang, H. Su & J. Zhang (2025). A systematic resilience assessment framework for multi-state systems based on physics-informed neural network. *Reliability Engineering & System Safety*, *257, Part B*, Article ID: 110866. https://doi.org/10.1016/j.ress.2025.110866.

[16] X. Li & J. Zheng (2005). A unified approach to the extremal trees for different indices. *MATCH Communications in Mathematical and in Computer Chemistry*, *54*(1), 195–208.

[17] H. Lv, J. Zeng, Z. Zhu, S. Dong & W. Li (2024). Study on prestress distribution and structural performance of heptagonal six-five-strut alternated cable dome with inner hole. *Structures*, *65*, Article ID: 106724. https://doi.org/10.1016/j.istruc.2024.106724.

M. Manuel and A. Parthiban

Malaysian J. Math. Sci. 20(1): 21–42(2026) 21 - 42

[18] A. Mohajeri, P. Manshour & M. Mousaee (2017). A novel topological descriptor based on the expanded Wiener index: applications to QSPR/QSAR studies. *Iranian Journal of Mathematical Chemistry*, *8*(2), 107–135. https://doi.org/10.22052/ijmc.2017.27307.1101.

[19] National Center for Biotechnology Information. PubChem Compound Summary. Technical report National Library of Medicine 2024. https://pubchem.ncbi.nlm.nih.gov.

[20] M. Randić (1975). Characterization of molecular branching. *Journal of the American Chemical Society*, *97*(23), 6609–6615. https://doi.org/10.1021/ja00856a001.

[21] Royal Society of Chemistry. ChemSpider Database. Technical report Royal Society of Chemistry 2024. https://www.chemspider.com.

[22] X. Sun & J. Du (2022). On Sombor index of trees with fixed domination number. *Applied Mathematics and Computation*, *421*, Article ID: 126946. https://doi.org/10.1016/j.amc.2022.126946.

[23] X. Sun, J. Du & Y. Mei (2024). Lower bound for the Sombor index of trees with a given total domination number. *Computational and Applied Mathematics*, *43*(6), Article ID: 356. https://doi.org/10.1007/s40314-024-02871-8.

[24] N. Trinajstic (2018). *Chemical Graph Theory*. CRC Press, Boca Raton, Florida.

[25] D. B. West et al. (2001). *Introduction to Graph Theory* volume 2. Prentice Hall, Upper Saddle River, New Jersey.

[26] Y. Wu & T. Shen (2017). A finite convergence criterion for the discounted optimal control of stochastic logical networks. *IEEE Transactions on Automatic Control*, *63*(1), 262–268. https://doi.org/10.1109/TAC.2017.2720730.

[27] X. Zhang, Y. Zhang, A. L. Chen, M. Yu & L. Zhang (2025). Optimizing multi label student performance prediction with GNN-TINet: A contextual multidimensional deep learning framework. *PloS One*, *20*(1), Article ID: e0314823. https://doi.org/10.1371/journal.pone.0314823.

[28] Y. Zhang, H. Wang, G. Su & K. C. Das (2024). Extremal problems on the Atom-bond sum-connectivity indices of trees with given matching number or domination number. *Discrete Applied Mathematics*, *345*, 190–206. https://doi.org/10.1016/j.dam.2023.11.046.

[29] D. Zheng & X. Cao (2025). Provably efficient service function chain embedding and protection in edge networks. *IEEE Transactions on Networking*, *33*(1), 178–193. https://doi.org/10.1109/TNET.2024.3475248.

[30] Y. Zhu, Y. Zhou, L. Yan, Z. Li, H. Xin & W. Wei (2024). Scaling graph neural networks for large-scale power systems analysis: empirical laws for emergent abilities. *IEEE Transactions on Power Systems*, *39*(6), 7445–7448. https://doi.org/10.1109/TPWRS.2024.3437651.