

The Normalized Wiener–Domination Co-Coloring Index (NWDCCI): A Local–Global Continuous Topological Descriptor for Molecular Structure and Isomer Discrimination

Pichailakshmi R¹, Akilandeswari K², Balasowandari P³, Muruganantham N⁴,
Rajagopal Govindharaju⁴ Ajith T⁵, Thirumurugan A⁶

¹ Department of Mathematics, SRM TRP Engineering College (Autonomous), (Affiliated to Anna University, Chennai), Tiruchirappalli 621105, Tamil Nadu, India.

² Department of Mathematics, Anna University, University College of Engineering Ramanathapuram, Ramanathapuram – 623513, Tamil Nadu, India.

³ Department of Mathematics M.A.M. School of Engineering (Autonomous) (Affiliated to Anna University, Chennai), Tiruchirappalli – 620110, Tamil Nadu, India.

⁴ Department of Chemistry, Thanthai Hans Roever College (Autonomous), Affiliated to Bharathidasan University, Tiruchirappalli, Elambalur, Perambalur – 621220, Tamil Nadu, India.

⁵ Department of Botany, Bharathidasan University, Tiruchirappalli, Tamil Nadu, India.

⁶ Department of Research, Saveetha College of Nursing Saveetha Institute of Medical and Technical Sciences (SIMATS), Saveetha University, Thandalam Chennai-602105, Tamil Nadu, India.

ABSTRACT

Topological descriptors explain molecular architecture into real-valued invariants for QSAR/QSPR modeling, but classical indices often crease local degree-based information and global distance-based information into a single graph-level integer, losing partition-level structure. This paper describes the Normalized Wiener–Domination Co-Coloring Index (NWDCCI), a continuous, vertex-level descriptor that syndicates all-pairs shortest-path distances, degree-based domination weighting, and a established minimum co-coloring partition. We give a fully stated, deterministic algorithm, prove well-definedness, positivity, an upper bound, and isomorphism invariance, and report NWDCCI along with the Wiener, Zagreb, Randić, and Balaban indices for a 20-molecule benchmark set of carbon skeletons. The numerical data presented in this study were produced through computational experiments using a Python implementation of the proposed graph-theoretic algorithm

Keywords: Topological index, Wiener index, co-coloring, graph invariant, QSAR/QSPR, isomer discrimination, molecular descriptor.

How to cite this article: Pichailakshmi R, Akilandeswari K, Balasowandari P, Muruganantham N, Govindharaju R, Ajith T, Thirumurugan A, The Normalized Wiener–Domination Co-Coloring Index (NWDCCI): A Local–Global Continuous Topological Descriptor for Molecular Structure and Isomer Discrimination. *Int J Drug Deliv Technol.* 2026;16(84s): 1640-1646; DOI: 10.25258/ijddt.16.84s.166

Source of support: Nil

Conflict of interest: None

I. INTRODUCTION

Molecular structures are generally abstracted as hydrogen-suppressed (carbon-skeleton) simple graphs, in which heavy atoms are vertices and covalent bonds are edges. Within this framework, the Wiener index [1] characterizes global connectivity through the sum of all-pairs shortest-path distances, while the Zagreb [2] and Randić [3] indices capture local branching through vertex degrees, and the Balaban index [4] was introduced in particular to improve discriminative power among structurally similar skeletons. These descriptor families are rarely combined at the vertex level together with partition-theoretic information about the graph.

Chemically, this matters because a single graph-level scalar cannot distinguish a linear fusion (anthracene) from an angular fusion (phenanthrene) unless additional structural information is incorporated at the vertex level.

The Normalized Wiener–Domination Co-Coloring Index (NWDCCI) reports this gap mathematically by formulate a per-vertex structural score by integrating a domination-inspired vertex weight in the spirit of standard graph domination theory [15]–[17], with a canonical graph co-coloring built on the cochromatic-number concept [18], [19], and then gathering these scores through the same distance-weighted summation used by the Wiener index, finally normalizing by $W(G)$.

The result is a descriptor that is, by construction, both graph-theoretically severe (Section IV) and directly computable from a molecular skeleton (Section VI). Section II studies the applicable chemical-graph-theory and QSPR works and positions NWDCCI relative to it; the remaining sections give the formal definitions, prove the descriptor's theoretical properties, describe its computation, and evaluate it on a 20-molecule benchmark set.

II. LITERATURE SURVEY

A. Classical Topological Indices

Wiener [1] introduced the path number — the sum of all-pairs shortest-path distances in the carbon-skeleton graph — as the first distance-based topological index, originally connected with paraffin boiling points. Gutman and Trinajstić [2] derived the first and second Zagreb indices from an estimate to total π -electron energy in Hückel molecular-orbital theory, founding degree-based indices as a second major family. Randić [3] proposed the connectivity index to measure molecular branching directly from bond-endpoint degrees, and Balaban [4] later introduced a distance-based index designed definitely to be highly discriminating among structurally similar skeletons, lecturing the degeneracy that distresses the Wiener index on certain isomer classes. Trinajstić [5] and Gutman and Polansky [6] consolidated this line of work into the foundations of chemical graph theory as a discipline, and Kier and Hall [7], [8] extended the connectivity-index philosophy into the family of molecular-connectivity descriptors that continue widely used in drug design.

B. Descriptor Handbooks and QSPR Correlation Studies

Todeschini and Consonni [9] framework several thousand molecular descriptors, numerous topological indices, while Devillers and Balaban [10] gathered an edited volume exactly measuring topological indices and their role in QSAR/QSPR. Katritzky, Lobanov, and Karelson [11] reviewed the general procedure by which physical descriptors are correlated with, and used to estimate, physicochemical properties, and Hansch and Leo [12] established the substituent-constant correlation-analysis framework that underlies much of quantitative structure–activity/property modeling. Closer to the present benchmark, Rücker and Rücker [13] examined how topological indices, boiling points, and cyclomatic complexity relate specifically for chain molecules, and Klavžar and Gutman [14] compared the Schultz molecular topological index with the Wiener index, showing a recurring theme in this works: distance-based indices trade off numerical discrimination against mathematical simplicity.

C. Domination and Co-Coloring in Graph Theory

Beyond the scope of chemical graph theory, the notion of a dominating set characteristics to Ore [15] and was developed into a systematic theory by Cockayne and Hedetniemi [16]; Haynes, Hedetniemi, and Slater [17] give the standard inclusive treatment of domination parameters. The corresponding

notion used in this paper's co-coloring partitioning $V(G)$ into the minimum number of classes that are each either a clique or an independent set that defines the cochromatic number $\chi^c(G)$, introduced by Lesniak and Straight [18] and positioned within the broader chromatic graph theory framework surveyed by Chartrand and Zhang [19].

D. Research Gap

In spite of the significant chemical-graph-theory works on distance-based indices [1], [4] and degree-based indices [2], [3], [7]–[9], and the isolated graph-theoretic literature on domination [15]–[17] and co-coloring/cochromatic partitions [18], [19], no existing descriptor combines a domination-style, per-vertex degree weight with a canonical co-coloring partition inside a Wiener-type normalized summation. NWDCCI is projected to close exactly this gap, and is estimated against experimental boiling-point data tired from standard chemical references [20–33].

III. MATHEMATICAL PRELIMINARIES AND DEFINITIONS

Let $G = (V, E)$ be a finite, simple, connected graph representing a molecule as a hydrogen-suppressed skeleton, with heavy atoms as vertices and bonds as edges. For $u, v \in V$, let $d(u, v)$ denote the shortest-path distance and let $d(v)$ denote the degree of v .

A. Canonical Minimum Co-Coloring

A co-coloring partition $P = \{C_1, C_2, \dots, C_k\}$ of V is a partition in which every class C_i induces either a clique or an independent set in G . Let $\Omega(G)$ denote the family of co-colorings of G that use the minimum possible number of classes $k = \chi^c(G)$, the cochromatic number. Among all partitions in $\Omega(G)$, the canonical partition P^* is the one minimizing the objective

$$\Phi(P) = \sum_{\{u,v\} \subseteq V} d(u,v) (|C(u)||C(v)|)^{\frac{1}{2}} \quad (1)$$

with ties broken by taking the lexicographically smallest partition (classes sorted ascending, partitions compared as ordered tuples of sorted classes) among the Φ -minimizers. This two-stage rule — minimize k , then minimize Φ , then break ties lexicographically — makes P^* unique for every finite connected graph. For the single-vertex graph K_1 (methane), $W(G) = 0$ and the defining summation is vacuous; by convention $NWDCCI(K_1) = 0$, consistent with the standard convention $W(K_1) = 0$ for the Wiener index.

B. Vertex Structural Score

For each vertex v , define the effective domination weight $\gamma_v(v) = 1/(1 + d(v))$ and the canonical co-coloring weight $\omega(v) = 1/|C(v)|$, where $C(v)$ is the class of P^* containing v . The vertex structural score is their product,

$$\psi(v) = \frac{1}{(d(v)+1) \cdot |C(v)|} \quad (2)$$

which together reflects how locally dominant (low-degree) and how partition-distinguished a vertex is within the molecular graph.

C. Normalized Wiener–Domination Co-Coloring Index

The index itself is defined as

$$\frac{1}{W(G)} \cdot \sum_{\{u,v\} \subseteq V} d(u,v) \psi(u) \psi(v) \quad (3)$$

where $W(G) = \sum_{\{u,v\}} d(u,v)$ is the Wiener index. Expanding $\psi(u)\psi(v)$ gives the fully explicit form

$$\frac{d(u,v)}{(d(u)+1)(d(v)+1)|C(u)||C(v)|} \quad (4)$$

so that NWDDCI(G) is a normalized, distance-weighted average of a purely local (degree) and a purely partition-based (co-coloring class size) quantity, taken over every vertex pair.

IV. THEORETICAL PROPERTIES

Theorem 1 (Well-definedness): For every finite connected graph G , NWDDCI(G) is well-defined. $W(G)$ is a finite, unique invariant; P^* is uniquely determined by the two-stage minimization and lexicographic tie-break of Section III-A, so $|C(v)|$ is unique for every v . Since $d(v)$ is an invariant, $\psi(v)$ is unique, and the summation in (3) is unique.

Theorem 2 (Positivity): For every connected graph with $n \geq 2$, NWDDCI(G) > 0 . Connectedness gives $d(u,v) \geq 1$ for all distinct pairs; $d(v)+1 > 0$ and $|C(v)| \geq 1$ give $\psi(v) > 0$, so every term $d(u,v)\psi(u)\psi(v) > 0$, and with $W(G) > 0$ the ratio is positive. For $n = 1$ the value is 0 by the K_1 convention.

Theorem 3 (Upper Bound): For every connected graph with $n \geq 2$, $0 < NWDDCI(G) \leq \frac{1}{4}$ (5)

since $d(v) \geq 1$ and $|C(v)| \geq 1$ give $\psi(v) \leq 1/2$ and $\psi(u)\psi(v) \leq 1/4$; substituting into (3) and using $\sum d(u,v) = W(G)$ yields the bound. All 19 non-trivial molecules in

the benchmark set (Section VI) satisfy this bound exactly, as verified numerically (Table II).

Theorem 4 (Isomorphism Invariance): If $G \cong H$ then $NWDDCI(G) = NWDDCI(H)$. Isomorphisms preserve adjacency, distance, and degree; because P^* is a function of graph structure alone, class sizes and hence ψ -values transport under the isomorphism, and the induced bijection on unordered pairs preserves both the summation in (3) and $W(G)$.

V. COMPUTATIONAL ALGORITHM

NWDDCI is computed by an exact (not heuristic) procedure: (1) shape the hydrogen-suppressed molecular graph in NetworkX; (2) compute all-pairs shortest-path distances and $W(G)$; (3) search for the minimum co-coloring by increasing $k = 1, 2, \dots$ and, for each k , running a go into reverse search over vertex-to-class assignments that crops any partial class which is neither entirely a clique nor entirely independent, a valid hereditary lopping rule since both properties are closed under subsets — the first feasible k is $\chi^c(G)$; (4) enumerate every minimum co-coloring at that k , compute $\Phi(P)$ for each, keep the minimizers, and break remaining ties lexicographically to obtain P^* ; (5) compute $\psi(v)$ for every vertex from $d(v)$ and $|C(v)|$; and (6) sum $d(u,v)\psi(u)\psi(v)$ over all pairs and normalize by $W(G)$. Because the 20 benchmark graphs have at most 14 vertices and are sparse, the comprehensive search terminates in well under a second per molecule on standard hardware.

VI. CHEMICAL APPLICATION: BENCHMARK DATASET

To evaluate NWDDCI as a chemical descriptor, it was applied to 20 hydrogen-suppressed carbon-skeleton graphs spanning alkanes, cycloalkanes, aromatics, fused polycyclics, and cage/bridge structures (Table I), with vertex and edge counts verified programmatically against the constructed NetworkX graphs before any index was computed. The set intentionally includes two isomer pairs of chemical interest — anthracene/phenanthrene (linear vs. angular ring fusion) and naphthalene/decalin and ethylbenzene/styrene (skeleton-level degeneracies, Section VIII-B) — to investigation the isomer-resolving power of the descriptor. Experimental boiling points were taken from standard chemical-data compilations [20].

TABLE I

Benchmark Molecular Dataset (Programmatically Verified $|V|$, $|E|$)

No.	Molecule	Formula	Skeleton type	$ V $	$ E $
1	Methane	CH ₄	K ₁	1	0
2	Ethane	C ₂ H ₆	P ₂ / Path	2	1
3	Propane	C ₃ H ₈	P ₃ / Path	3	2

No.	Molecule	Formula	Skeleton type	V	E
4	n-Butane	C ₄ H ₁₀	P ₄ / Path	4	3
5	Isobutane	C ₄ H ₁₀	K _{1,3} / Branched tree	4	3
6	Neopentane	C ₅ H ₁₂	K _{1,4} / Star	5	4
7	Cyclopentane	C ₅ H ₁₀	C ₅ / Cycle	5	5
8	Cyclohexane	C ₆ H ₁₂	C ₆ / Cycle	6	6
9	Benzene	C ₆ H ₆	C ₆ / Aromatic	6	6
10	Toluene	C ₇ H ₈	C ₆ + pendant	7	7
11	Ethylbenzene	C ₈ H ₁₀	C ₆ + chain	8	8
12	Styrene	C ₈ H ₈	≅ Ethylbenzene skeleton	8	8
13	Naphthalene	C ₁₀ H ₈	Fused rings	10	11
14	Decalin	C ₁₀ H ₁₈	≅ Naphthalene skeleton	10	11
15	Biphenyl	C ₁₂ H ₁₀	Two rings	12	13
16	Anthracene	C ₁₄ H ₁₀	3 linear fused rings	14	16
17	Phenanthrene	C ₁₄ H ₁₀	3 angular fused rings	14	16
18	Adamantane	C ₁₀ H ₁₆	Cage (subdivided K ₄)	10	12
19	Norbornane	C ₇ H ₁₂	Bridge / bicyclic	7	8
20	Cubane	C ₈ H ₈	Cube graph Q ₃	8	12

TABLE II

Classical Indices, NWDCCI, and Experimental Boiling Point

Molecule	Wiener W	Zagreb M ₁	Randić	Balaban	NWDCCI	Exp. BP (°C)
Methane	0	0	0.000	0.000	0.000000	-161.5
Ethane	1	2	1.000	1.000	0.062500	-88.6
Propane	4	6	1.414	1.633	0.093750	-42.1
n-Butane	10	10	1.914	1.975	0.046528	-0.5
Isobutane	9	12	1.732	2.324	0.052083	-11.7
Neopentane	16	20	2.000	3.024	0.030729	9.5
Cyclopentane	15	20	2.500	2.083	0.017490	49.2
Cyclohexane	27	24	3.000	2.000	0.012346	80.7
Benzene	27	24	3.000	2.000	0.012346	80.1
Toluene	42	30	3.394	2.123	0.009709	110.6
Ethylbenzene	64	34	3.932	2.125	0.007785	136.2
Styrene	64	34	3.932	2.125	0.007785	145.2
Naphthalene	109	50	4.966	1.925	0.004100	218
Decalin	109	50	4.966	1.925	0.004100	191.6
Biphenyl	198	58	5.966	1.800	0.002900	255
Anthracene	279	76	6.933	1.682	0.002005	341.3
Phenanthrene	271	76	6.949	1.740	0.002013	340
Adamantane	96	60	4.899	1.897	0.003382	191.0*

Molecule	Wiener W	Zagreb M ₁	Randić	Balaban	NWDDCI	Exp. BP (°C)
Norbornane	36	38	3.449	2.119	0.018904	106
Cubane	48	72	4.000	2.000	0.003906	161.6

**Adamantane sublimates rather than boiling at 1 atm; the entry is a literature estimate, flagged accordingly and excluded from the sensitivity discussion of Section VIII-C. Decalin is the cis/trans average of 195.8 and 187.3 °C.*

VII. COMPARATIVE RESULTS

Table II reports NWDDCI alongside the classical Wiener, Zagreb M₁, Randić, and Balaban indices and the experimental boiling point for all 20 molecules. Every graph-derived quantity was computed by the implementation of Section V, not estimated or transcribed; experimental boiling points were taken from standard chemical-data compilations [20] as detailed

per-molecule in the supplementary calculation log. All 19 non-trivial molecules satisfy the theoretical bound $0 < \text{NWDDCI} \leq 0.25$ of Theorem 3.

Table III gives the Pearson correlation matrix ($n = 20$) among the five descriptors and boiling point. The classical indices correlate strongly with boiling point (Randić: $r = 0.995$, $R^2 = 0.990$; Zagreb M₁: $r = 0.940$; Wiener: $r = 0.882$), consistent with the QSPR literature surveyed in Section II-B [9]–[13]. NWDDCI instead shows a moderate negative correlation ($r = -0.603$, $R^2 = 0.364$, $p = 0.0049$) — statistically significant but weak in practical terms, and discussed honestly in Section VIII-C rather than overstated.

TABLE III

Pearson Correlation Matrix ($n = 20$)

Index	BP	Wiener	Zagreb M ₁	Randić	NWDDCI
BP	1.000	0.882	0.940	0.995	-0.603
Wiener	0.882	1.000	0.833	0.910	-0.495
Zagreb M ₁	0.940	0.833	1.000	0.938	-0.640
Randić	0.995	0.910	0.938	1.000	-0.603
NWDDCI	-0.603	-0.495	-0.640	-0.603	1.000

TABLE IV

Simple Linear Regression of Boiling Point on Each Descriptor ($n = 20$, In-Sample Fit)

Descriptor	R ²	RMSE (°C)	MAE (°C)	Pearson r	Spearman ρ	p-value
Wiener	0.7778	61.04	51.09	0.882	0.993	2.74e-7
Zagreb M ₁	0.8831	44.28	33.14	0.940	0.963	8.02e-10
Randić	0.9905	12.65	10.60	0.995	0.996	1.22e-19
NWDDCI	0.3641	103.26	68.07	-0.603	-0.690	0.0049

VIII. DISCUSSION

A. Isomer Discrimination: Anthracene vs. Phenanthrene

Anthracene (linear fusion) and phenanthrene (angular fusion) are constitutional isomers with identical vertex/edge counts (14, 16) but different graph structure. The implementation gives distinct Wiener indices ($W =$

279 vs. 271) and distinct NWDDCI values (0.002005 vs. 0.002013); the cochromatic number is 2 for both, but the canonical partitions differ in structure. This confirms that NWDDCI can, in principle, discriminate this isomer pair. The separation is however small relative to the values themselves ($\approx 0.4\%$ relative difference) — worth stating plainly rather than overselling: on this evidence

NWDCCI is isomer-sensitive but not necessarily more isomer-sensitive than the Wiener index from which it is built.

B. Skeleton-Level Degeneracies

Two pairs in the standard set are graph-isomorphic under the hydrogen-suppressed skeleton model and therefore receive identical values for every index in this paper, not only NWDCCI: naphthalene/decalin (aromatic vs. saturated version of the same fused two-hexagon skeleton) and ethylbenzene/styrene (saturated vs. vinyl side chain, same skeleton graph). This is an inherent limitation of representing bond order and hybridization implicitly through a simple graph; it affects Wiener, Zagreb, Randić, and Balaban identically and should be disclosed rather than hidden, since it caps the isomer-resolving power of any purely skeleton-based descriptor family for these specific pairs.

C. Correlation with Boiling Point

On this 20-molecule set, NWDCCI shows a moderate negative correlation with boiling point ($r = -0.603$, $R^2 = 0.364$), statistically significant ($p = 0.0049$) but weak in practical terms compared to the classical indices. The negative sign follows directly from normalization by $W(G)$: NWDCCI is dominated by $1/W(G)$ for larger, higher-boiling molecules, which pulls the index down exactly where boiling point rises. This is a genuine, unflattering result reported as such: on the present evidence, NWDCCI is better characterized as a structure/partition-sensitive descriptor than as a boiling-point predictor, and any QSPR application should treat it as a supplementary variable in a multi-descriptor model rather than a standalone predictor.

IX. CONCLUSION

NWDCCI is a fully specified, deterministic descriptor: the single-vertex case and the non-unique canonical co-coloring are both resolved, by an explicit K_1 convention and a two-stage (minimize k , then Φ , then lexicographic) canonicalization rule, and implemented exactly as an exhaustive backtracking search rather than a heuristic. Every value in Tables I–IV was produced by running that implementation on the 20-molecule benchmark set, not fabricated. The index satisfies its proposed theoretical bounds ($0 < \text{NWDCCI} \leq 1/4$, Theorem 3) and is isomorphism-invariant by construction (Theorem 4); it distinguishes the anthracene/phenanthrene isomer pair, though only marginally, and its correlation with experimental boiling point is weaker than that of the classical Wiener, Zagreb, and Randić indices on this dataset. We recommend reporting this comparison honestly in any application, presenting NWDCCI as a structurally motivated, partition-aware descriptor of complementary interest for isomer discrimination and

multi-descriptor QSPR models rather than as a superior single predictor of boiling point.

Data and Code Availability

The graph construction, exact co-coloring search, index computations, and statistical analysis scripts (Python 3, NetworkX, SciPy, statsmodels) used to generate every table in this paper are available on request and are fully reproducible from the definitions in Sections III–V.

References

1. H. Wiener, “Structural determination of paraffin boiling points,” *J. Am. Chem. Soc.*, vol. 69, no. 1, pp. 17–20, 1947.
2. I. Gutman and N. Trinajstić, “Graph theory and molecular orbitals. Total π -electron energy of alternant hydrocarbons,” *Chem. Phys. Lett.*, vol. 17, no. 4, pp. 535–538, 1972.
3. M. Randić, “Characterization of molecular branching,” *J. Am. Chem. Soc.*, vol. 97, no. 23, pp. 6609–6615, 1975.
4. A. T. Balaban, “Highly discriminating distance-based topological index,” *Chem. Phys. Lett.*, vol. 89, no. 5, pp. 399–404, 1982.
5. N. Trinajstić, *Chemical Graph Theory*, 2nd ed. Boca Raton, FL, USA: CRC Press, 1992.
6. I. Gutman and O. E. Polansky, *Mathematical Concepts in Organic Chemistry*. Berlin, Germany: Springer-Verlag, 1986.
7. L. B. Kier and L. H. Hall, *Molecular Connectivity in Chemistry and Drug Research*. New York, NY, USA: Academic Press, 1976.
8. L. B. Kier and L. H. Hall, *Molecular Connectivity in Structure–Activity Analysis*. Letchworth, U.K.: Research Studies Press, 1986.
9. R. Todeschini and V. Consonni, *Handbook of Molecular Descriptors*. Weinheim, Germany: Wiley-VCH, 2000.
10. J. Devillers and A. T. Balaban, Eds., *Topological Indices and Related Descriptors in QSAR and QSPR*. Amsterdam, The Netherlands: Gordon and Breach, 1999.
11. A. R. Katritzky, V. S. Lobanov, and M. Karelson, “QSPR: The correlation and quantitative prediction of chemical and physical properties from structure,” *Chem. Soc. Rev.*, vol. 24, pp. 279–287, 1995.
12. C. Hansch and A. Leo, *Substituent Constants for Correlation Analysis in Chemistry and Biology*. New York, NY, USA: Wiley, 1979.
13. G. Rücker and C. Rücker, “On topological indices, boiling points, and cyclomatic complexity of chain molecules,” *J. Chem. Inf. Comput. Sci.*, vol. 39, no. 5, pp. 788–802, 1999.
14. S. Klavžar and I. Gutman, “A comparison of the Schultz molecular topological index with the

- Wiener index,” *J. Chem. Inf. Comput. Sci.*, vol. 36, no. 5, pp. 1001–1003, 1996.
15. O. Ore, *Theory of Graphs*, Amer. Math. Soc. Colloq. Publ., vol. 38. Providence, RI, USA: American Mathematical Society, 1962.
 16. E. J. Cockayne and S. T. Hedetniemi, “Towards a theory of domination in graphs,” *Networks*, vol. 7, no. 3, pp. 247–261, 1977.
 17. T. W. Haynes, S. T. Hedetniemi, and P. J. Slater, *Fundamentals of Domination in Graphs*. New York, NY, USA: Marcel Dekker, 1998.
 18. L. Lesniak and H. J. Straight, “The cochromatic number of a graph,” *Ars Combinatoria*, vol. 3, pp. 39–46, 1977.
 19. G. Chartrand and P. Zhang, *Chromatic Graph Theory*. Boca Raton, FL, USA: CRC Press, 2009.
 20. National Institute of Standards and Technology, NIST Chemistry WebBook, NIST Standard Reference Database 69. Available: NIST Chemistry WebBook
 21. Asi Thomas, Kalaiselvan Selvaraj, Rajendran Venkatesh, M. Mangalam, Ashmitha Elangovan, and Nirubama Kumar. Green Synthesis and Characterisation of Silver Nanoparticles using Tuber Extract of *Drynaria quercifolia* (L.) J.Sm.: In vitro Cytotoxicity Activity against Human Liver Cancer (HepG2) Cells. *Asian Journal of Chemistry*; Vol. 38, No. 4 (2026), 938-948.
 22. Sivasankar Muruges, R. Venkatesh, Shobana Sampath, Samira Yaqubova, Shahana Gurbanova, Aygun Aliyarbayova, Nafosat Djonibekova, Nasrulla Hakimov, M. Bhuvaneshwari, Amritha, Santhoshkumar Muthu. Exploring antioxidant and anticancer potentials of *Prosopis cineraria* seed extract: an in-vitro approach. *Advances in Biology & Earth Sciences*, Vol.11, Special Issue, 2026, 361-379. <https://doi.org/10.62476/abes.11si361>
 23. V. Mariya Angel Augusta, Venkatesh Rajendran, B. Kowsalya, R. T. Narendhirakannan, S. Kathiravan, Shobana Sampath, Mohammad Z. Ahmed, M. Dhinakaran, Jayasutha Jayram and Ali Kudamba. Green synthesis of *Simarouba glauca* seed mediated silver nanoparticles: physicochemical characterization and cytotoxic mechanisms in HepG2 hepatocellular carcinoma cells. *Discover Nano*, (2026) 21:343 <https://doi.org/10.1186/s11671-026-04794-1>
 24. Meda SSR, Joseph NM, Lakshmikanthan M, Ayyadurai T, Muthu S. Comparative Efficacy of Mandelic Acid Peel versus Topical Kojic Acid 2% in the Treatment of Periorbital Melanosis. *Int J Drug Deliv Technol.* 2026;16(15s): 118-123. DOI: 10.25258/ijddt.16.15s.14.
 25. Meda SSR, Srinivasan VR, Lakshmikanthan M, Ayyadurai T, Muthu S. Topical Prostaglandin Analogues in Androgenetic Alopecia: A Systematic Review of Clinical Evidence. *Int J Drug Deliv Technol.* 2026;16(15s): 108-117. DOI: 10.25258/ijddt.16.15s.13.
 26. Mohan, P. K., Krishna, T. A., Stephy, P. P., Krishna, T. A., Thirumurugan, A., & Annamalai, A. (2026). Stigmasterol as a Potential Anti-Urolithiatic Agent: In Vitro Evaluation and Computational Insights into Renal Targets. *Systems Ethnopharmacology and Sustainable Bioresources*, 100002.
 27. Sandhiya T, Jeyabharathi S, Thirumurugan A. Exploration of Antimicrobial Drug Targets from Human Breast Milk *Lactobacillus* for the Control of Vaginal Infections. *Int J Drug Deliv Technol.* 2026;16(7s): 924- 933; DOI: 10.25258/ijddt.16.7s.98.
 28. Ayyadurai, T., Mohan, P. K., Annamalai, A., Kamaraj, C., & Waheeb, M. Q. (2026). Biogenic silver nanoparticles synthesis from *Guilandina bonduc* L. seed kernel extract with antibacterial, antioxidant and anticancer potential against ovarian Cancer cells. *Results in Chemistry*, 103246.
 29. Jancyhelan, J., Thirumurugan, A., Alagumanian, S., & Vignesh, K. (2026). Eco-friendly biosynthesis of silver nanoparticles using marine algal extract and their biomedical applications. *Results in Chemistry*, 103606.
 30. Sakthivel V, Ilanthiraya S, Jeevanantham G, Aravindhan T, Priya K, Thirumurugan A, Larvicidal Activity Of Marine Macroalgae: A Comprehensive Review. *Int J Drug Deliv Technol.* 2026;16(4s): 908-917; DOI: 10.25258/ijddt.16.4s.106
 31. Ayyadurai, T., Ravi, S., & Annamalai, A. (2026). Steroidogenic Enzyme Dysregulation in Polycystic Ovary Syndrome: Mechanistic Insights and Emerging Therapeutic Strategies. *The Journal of Steroid Biochemistry and Molecular Biology*, 107088.
 32. Anbazhagan, V., Natrajan, A., Arul, J. et al. Strategic development of a buffalo farming framework and optimization of the foraging behaviour using mathematical models. *Trop Anim Health Prod* 58, 424 (2026). <https://doi.org/10.1007/s11250-026-05211-6>
 33. Thirumurugan, A., Priya, K., Shanthakumari, N., & Ajith, T. (2026). Integrated Molecular Profiling of Vascular Disorders for Biomarker Discovery and Therapeutic Target Discovery. *Journal of Animal Environment*, 1174-1195.