Bibliography

[1] F. Harary, *Graph theory.* Addison-Wesley publishing company, 1969.

[2] N. Trinajstic, *Chemical graph theory.* CRC press, 2018.

[3] D. Bonchev, *Information theoretic indices for characterization of chemical structures.* Research Studies Press, Chichester, U. K, 1983.

[4] C. E. Shannon and W. Weaver, "The mathematical theory of communication," 1949.

[5] J. Bondy and U. Murty, *Graph theory with applications*, vol. 244. Springer-Verlag London, 2008.

[6] M. Grover, B. Singh, M. Bakshi, and S. Singh, "Quantitative structure–property relationships in pharmaceutical research–part 1," *Pharmaceutical science & technology today*, vol. 3, no. 1, pp. 28–35, 2000.

[7] I. Gutman and Ž. Tomović, "Relation between distance-based topological indices," *Journal of chemical information and computer sciences*, vol. 40, no. 6, pp. 1333–1336, 2000.

[8] H. Wiener, "Structural determination of paraffin boiling points," *Journal of the American Chemical Society*, vol. 69, no. 1, pp. 17–20, 1947.

[9] A. A. Dobrynin, R. Entringer, and I. Gutman, "Wiener index of trees: theory and applications," *Acta Applicandae Mathematica*, vol. 66, no. 3, pp. 211–249, 2001.

[10] A. A. Dobrynin, I. Gutman, S. Klavžar, and P. Žigert, "Wiener index of hexagonal systems," *Acta Applicandae Mathematica*, vol. 72, no. 3, pp. 247–294, 2002.

[11] A. Graovac and T. Pisanski, "On the Wiener index of a graph," *Journal of mathematical chemistry*, vol. 8, no. 1, pp. 53–62, 1991.

[12] I. Gutman, "Some properties of the Wiener polynomial," *Graph Theory Notes New York*, vol. 125, pp. 13–18, 1993.

[13] S. Klavzar, I. Gutman, and B. Mohar, "Labeling of benzenoid systems which reflects the vertex-distance relations," *Journal of chemical information and computer sciences*, vol. 35, no. 3, pp. 590–593, 1995.

[14] R. Škrekovski and I. Gutman, "Vertex version of the Wiener theorem," *MATCH Commun. Math. Comput. Chem*, vol. 72, no. 1, pp. 295–300, 2014.

[15] S. Nikolić and N. Trinajstić, "The Wiener index: Development and applications," *Croatica Chemica Acta*, vol. 68, no. 1, pp. 105–129, 1995.

[16] A. R. Ashrafi and S. Yousefi, "Computing the Wiener index of a TUC4C8 (S) nanotorus," *MATCH Commun. Math. Comput. Chem*, vol. 57, no. 2, pp. 403–10, 2007.

[17] V. Chepoi and S. Klavžar, "The Wiener index and the Szeged index of benzenoid systems in linear time," *Journal of chemical information and computer sciences*, vol. 37, no. 4, pp. 752–755, 1997.

[18] S. Yousefi and A. R. Ashrafi, "An exact expression for the Wiener index of a polyhex nanotorus," *MATCH Commun. Math. Comput. Chem*, vol. 56, no. 1, pp. 169–178, 2006.

[19] H. Liu and X.-F. Pan, "On the Wiener index of trees with fixed diameter," *MATCH Commun. Math. Comput. Chem*, vol. 60, no. 1, pp. 85–94, 2008.

[20] S. G. Wagner, "A class of trees and its Wiener index," *Acta Applicandae Mathematica*, vol. 91, no. 2, pp. 119–132, 2006.

[21] M. Randić, "On generalization of Wiener index for cyclic structures," *Acta Chim. Slov*, vol. 49, no. 3, pp. 483–496, 2002.

[22] I. Gutman and S. Klavzar, "Relations between Wiener numbers of benzenoid hydrocarbons and phenylenes," *Models in Chemistry*, vol. 135, no. 1, pp. 45–56, 1998.

[23] I. Gutman and B. Furtula, "A survey on terminal Wiener index," *Novel Molecular Structure Descriptors-Theory and Applications I, Univ. Kragujevac, Kragujevac*, vol. 173, p. 190, 2010.

[24] K. Xu, M. Liu, K. C. Das, I. Gutman, and B. Furtula, "A survey on graphs extremal with respect to distance-based topological indices," *MATCH Commun. Math. Comput. Chem*, vol. 71, no. 3, pp. 461–508, 2014.

[25] M. Randić, "Novel molecular descriptor for structure—property studies," *Chemical Physics Letters*, vol. 211, no. 4-5, pp. 478–483, 1993.

[26] D. J. Klein, I. Lukovits, and I. Gutman, "On the definition of the hyper-Wiener index for cycle-containing structures," *Journal of chemical information and computer sciences*, vol. 35, no. 1, pp. 50–52, 1995.

[27] M. Khalifeh, H. Yousefi-Azari, and A. R. Ashrafi, "The hyper-Wiener index of graph operations," *Computers & Mathematics with Applications*, vol. 56, no. 5, pp. 1402–1407, 2008.

[28] M.-h. Liu and B. Liu, "Trees with the seven smallest and fifteen greatest hyper-Wiener indices," *MATCH Commun. Math. Comput. Chem*, vol. 63, pp. 151–170, 2010.

[29] I. Gutman and B. Furtula, "Hyper-Wiener index vs. Wiener index. Two highly correlated structure-descriptors," *Monatshefte für Chemie/Chemical Monthly*, vol. 134, no. 7, pp. 975–981, 2003.

[30] I. Gutman, "Relation between hyper-Wiener and Wiener index," *Chemical physics letters*, vol. 364, no. 3-4, pp. 352–356, 2002.

[31] B. Zhou and I. Gutman, "Relations between Wiener, hyper-Wiener and Zagreb indices," *Chemical Physics Letters*, vol. 394, no. 1-3, pp. 93–95, 2004.

[32] S. Klavžar and I. Gutman, "Relation between Wiener-type topological indices of benzenoid molecules," *Chemical physics letters*, vol. 373, no. 3-4, pp. 328–332, 2003.

[33] K. C. Das, I. Gutman, and B. Furtula, "Survey on geometric-arithmetic indices of graphs," *MATCH Commun. Math. Comput. Chem*, vol. 65, no. 3, pp. 595–644, 2011.

[34] K. C. Das, M. A. Mohammed, I. Gutman, and K. A. Atan, "Comparison between atom-bond connectivity indices of graphs," *MATCH Commun. Math. Comput. Chem*, vol. 76, no. 1, pp. 159–170, 2016.

[35] T. Došlic, B. Furtula, A. Graovac, I. Gutman, S. Moradi, and Z. Yarahmadi, "On vertex–degree–based molecular structure descriptors," *MATCH Commun. Math. Comput. Chem*, vol. 66, no. 2, pp. 613–626, 2011.

[36] E. Estrada, "The ABC matrix," *Journal of Mathematical Chemistry*, vol. 55, no. 4, pp. 1021–1033, 2017.

[37] B. Furtula, I. Gutman, and M. Dehmer, "On structure-sensitivity of degree-based topological indices," *Applied Mathematics and Computation*, vol. 219, no. 17, pp. 8973–8978, 2013.

[38] W. Gao, M. K. Jamil, and M. R. Farahani, "The hyper-Zagreb index and some graph operations," *Journal of Applied Mathematics and Computing*, vol. 54, no. 1, pp. 263–275, 2017.

[39] I. Gutman, "Degree-based topological indices," *Croatica Chemica Acta*, vol. 86, no. 4, pp. 351–361, 2013.

[40] I. Gutman, B. Furtula, and C. Elphick, "Three new/old vertex-degree-based topological indices," *MATCH Commun. Math. Comput. Chem*, vol. 72, no. 3, pp. 617–632, 2014.

[41] M. Karelson, *Molecular descriptors in QSAR/QSPR*. Wiley-Interscience, 2000.

[42] S. Klavžar and I. Gutman, "Wiener number of vertex-weighted graphs and a chemical application," *Discrete applied mathematics*, vol. 80, no. 1, pp. 73–81, 1997.

[43] S. Klavžar and M. J. Nadjafi-Arani, "Wiener index in weighted graphs via unification of θ^*-classes," *European Journal of Combinatorics*, vol. 36, pp. 71–76, 2014.

[44] M. Liu and B. Liu, "A survey on recent results of variable Wiener index," *MATCH Commun. Math. Comput. Chem*, vol. 69, no. 3, pp. 491–520, 2013.

[45] J.-B. Liu, S. Wang, C. Wang, and S. Hayat, "Further results on computation of topological indices of certain networks," *IET Control Theory & Applications*, vol. 11, no. 13, pp. 2065–2071, 2017.

[46] S. Nikolić, G. Kovačević, A. Miličević, and N. Trinajstić, "The Zagreb indices 30 years after," *Croatica chemica acta*, vol. 76, no. 2, pp. 113–124, 2003.

[47] M. Randić, "On history of the Randić index and emerging hostility toward chemical graph theory," *MATCH Commun. Math. Comput. Chem*, vol. 59, no. 5, 2008.

[48] R. Todeschini and V. Consonni, *Handbook of molecular descriptors*, vol. 11. John Wiley & Sons, 2008.

[49] M. Randić, "Characterization of molecular branching," *Journal of the American Chemical Society*, vol. 97, no. 23, pp. 6609–6615, 1975.

[50] X. Li and Y. Shi, "A survey on the Randic index," *MATCH Commun. Math. Comput. Chem*, vol. 59, no. 1, pp. 127–156, 2008.

[51] X. Li, I. Gutman, and M. Randić, *Mathematical aspects of Randić-type molecular structure descriptors*. University, Faculty of Science, 2006.

[52] G. Caporossi, I. Gutman, P. Hansen, and L. Pavlović, "Graphs with maximum connectivity index," *Computational biology and chemistry*, vol. 27, no. 1, pp. 85–90, 2003.

[53] P. Yu, "An upper bound on the Randic index of trees," *J. Math. Study*, vol. 31, pp. 225–230, 1998.

[54] P. Hansen and H. Mélot, "Variable neighborhood search for extremal graphs. 6. Analyzing bounds for the connectivity index," *Journal of chemical information and computer sciences*, vol. 43, no. 1, pp. 1–14, 2003.

[55] H. Zhao and X. Li, "Trees with small Randić connectivity indices," *MATCH Commun Math. Comput. Chem. v51*, pp. 167–178, 2004.

[56] S. Fajtlowicz, "On conjectures of Graffiti-II," *Congr. Numer*, vol. 60, pp. 187–197, 1987.

[57] O. Favaron, M. Mahéo, and J.-F. Saclé, "Some eigenvalue properties in graphs: Conjectures of Graffiti—II)," *Discrete Mathematics*, vol. 111, no. 1-3, pp. 197–220, 1993.

[58] I. Gutman and N. Trinajstić, "Graph theory and molecular orbitals. total φ-electron energy of alternant hydrocarbons," *Chemical Physics Letters*, vol. 17, no. 4, pp. 535–538, 1972.

[59] I. Gutman and K. C. Das, "The first Zagreb index 30 years after," *MATCH Commun. Math. Comput. Chem*, vol. 50, no. 1, pp. 83–92, 2004.

[60] I. Gutman, E. Milovanović, and I. Milovanović, "Beyond the Zagreb indices," *AKCE International Journal of Graphs and Combinatorics*, no. 2, pp. 307–312, 2018.

[61] K. C. Das and I. Gutman, "Some properties of the second Zagreb index," *MATCH Commun. Math. Comput. Chem*, vol. 52, no. 1, pp. 3–1, 2004.

[62] C. M. da Fonseca and D. Stevanovic, "Further properties of the second Zagreb index," *MATCH Commun. Math. Comput. Chem*, vol. 72, pp. 655–668, 2014.

[63] J. Hao, "Theorems about Zagreb indices and modified Zagreb indices," *MATCH Commun. Math. Comput. Chem*, vol. 65, pp. 659–670, 2011.

[64] G. Shirdel, H. Rezapour, and A. Sayadi, "The hyper-Zagreb index of graph operations," *Iranian Journal of Mathematical Chemistry*, vol. 4, no. 2, pp. 213–220, 2013.

[65] B. Basavanagoud and S. Patil, "A note on hyper-Zagreb index of graph operations," *Iranian Journal of Mathematical Chemistry*, vol. 7, no. 1, pp. 89–92, 2016.

[66] B. Furtula, A. Graovac, and D. Vukičević, "Augmented Zagreb index," *Journal of mathematical chemistry*, vol. 48, no. 2, pp. 370–380, 2010.

[67] A. Miličević, S. Nikolić, and N. Trinajstić, "On reformulated Zagreb indices," *Molecular diversity*, vol. 8, no. 4, pp. 393–399, 2004.

[68] D. Vukičević and M. Gašperov, "Bond additive modeling 1. Adriatic indices," *Croatica chemica acta*, vol. 83, no. 3, pp. 243–260, 2010.

[69] A. Ali, S. Elumalai, and T. Mansour, "On the symmetric division deg index of molecular graphs," *MATCH Commun. Math. Comput. Chem*, vol. 83, pp. 205–220, 2020.

[70] C. Gupta, V. Lokesha, S. B. Shetty, and P. Ranjini, "Graph operations on symmetric division deg index of graphs," *Palestine Journal of Mathematics*, vol. 6, no. 1, pp. 280–286, 2017.

[71] C. Gupta, V. Lokesha, S. B. Shwetha, and P. Ranjini, "On the symmetric division deg index of graph.," *Southeast Asian Bulletin of Mathematics*, vol. 40, no. 1, 2016.

[72] C. Liu, Y. Pan, and J. Li, "Tricyclic graphs with the minimum symmetric division deg index," *Discr. Math. Lett*, vol. 3, pp. 14–18, 2020.

[73] V. Lokesha and T. Deepika, "Symmetric division deg index of tricyclic and tetracyclic graphs," *Int. J. Sci. Eng. Res*, vol. 7, no. 5, pp. 53–55, 2016.

[74] S. Naduvath, *Contemporary Studies in Discrete Mathematics*, vol. 2. Sudev Naduvath, 2018.

[75] Y. Pan and J. Li, "Graphs that minimizing symmetric division deg index," *MATCH Commun. Math. Comput. Chem*, vol. 82, no. 1, pp. 43–55, 2019.

[76] A. Vasilyev, "Upper and lower bounds of symmetric division deg index," *Iranian Journal of Mathematical Chemistry*, vol. 5, no. 2, pp. 91–98, 2014.

[77] B. Furtula and I. Gutman, "A forgotten topological index," *Journal of Mathematical Chemistry*, vol. 53, no. 4, pp. 1184–1190, 2015.

[78] M. O. Albertson, "The irregularity of a graph," *Ars Combinatoria*, vol. 46, pp. 219–225, 1997.

[79] I. Gutman, M. Togan, A. Yurttas, A. S. Cevik, and I. N. Cangul, "Inverse problem for sigma index," *MATCH Commun. Math. Comput. Chem*, vol. 79, no. 2, pp. 491–508, 2018.

[80] S. C. Basak, K. Balasubramanian, B. D. Gute, D. Mills, A. Gorczynska, and S. Roszak, "Prediction of cellular toxicity of halocarbons from computed chemodescriptors: A hierarchical QSAR approach," *Journal of chemical information and computer sciences*, vol. 43, no. 4, pp. 1103–1109, 2003.

[81] P. K. Chattaraj, *Chemical reactivity theory: a density functional view.* CRC press, 2009.

[82] S. C. Basak, D. Mills, and M. Mumtaz, "A quantitative structure–activity relationship (QSAR) study of dermal absorption using theoretical molecular descriptors," *SAR and QSAR in Environmental Research*, vol. 18, no. 1-2, pp. 45–55, 2007.

[83] J. Cioslowski, "Additive nodal increments for approximate calculation of the total π-electron energy of benzenoid hydrocarbons," *Theoretica chimica acta*, vol. 68, no. 4, pp. 315–319, 1985.

[84] J.-i. Aihara and M. Makino, "Constrained clar formulas of coronoid hydrocarbons," *The Journal of Physical Chemistry A*, vol. 118, no. 7, pp. 1258–1266, 2014.

[85] M. Arockiaraj, J. Clement, and K. Balasubramanian, "Analytical expressions for topological properties of polycyclic benzenoid networks," *Journal of Chemometrics*, vol. 30, no. 11, pp. 682–697, 2016.

[86] A. Behmaram, H. Yousefi-Azari, and A. Ashrafi, "Wiener polarity index of fullerenes and hexagonal systems," *Applied Mathematics Letters*, vol. 25, no. 10, pp. 1510–1513, 2012.

[87] J. R. Dias, "Structure and electronic characteristics of coronoid polycyclic aromatic hydrocarbons as potential models of graphite layers with hole defects," *The Journal of Physical Chemistry A*, vol. 112, no. 47, pp. 12281–12292, 2008.

[88] W. Gao and M. R. Farahani, "Computing the reverse eccentric connectivity index for certain family of nanocone and fullerene structures," *Journal of Nanotechnology*, vol. 2016, 2016.

[89] M. Ghorbani and M. Ghazi, "Computing some topological indices of triangular benzenoid," *Digest. J. Nanomater. Bios*, vol. 5, no. 4, pp. 1107–1111, 2010.

[90] S. Hayat and M. Imran, "Computation of topological indices of certain networks," *Applied Mathematics and Computation*, vol. 240, pp. 213–228, 2014.

[91] A. W. Bharati Rajan, C. Grigorious, and S. Stephen, "On certain topological indices of silicate, honeycomb and hexagonal networks," *Journal of Computer and Mathematical Sciences Vol*, vol. 3, no. 5, pp. 498–556, 2012.

[92] W. Gao, W. Wang, and M. R. Farahani, "Topological indices study of molecular structure in anticancer drugs," *Journal of chemistry*, vol. 2016, 2016.

[93] W. Gao, M. K. Siddiqui, M. Imran, M. K. Jamil, and M. R. Farahani, "Forgotten topological index of chemical structure in drugs," *Saudi pharmaceutical journal*, vol. 24, no. 3, pp. 258–264, 2016.

[94] W. Gao, Y. Wang, W. Wang, and L. Shi, "The first multiplication atom-bond connectivity index of molecular structures in drugs," *Saudi pharmaceutical journal*, vol. 25, no. 4, pp. 548–555, 2017.

[95] W. Gao, H. Wu, M. K. Siddiqui, and A. Q. Baig, "Study of biological networks using graph theory," *Saudi journal of biological sciences*, vol. 25, no. 6, pp. 1212–1219, 2018.

[96] A. T. Balaban, I. Motoc, D. Bonchev, and O. Mekenyan, "Topological indices for structure-activity correlations," in *Steric effects in drug design*, pp. 21–55, Springer, 1983.

[97] B. Liu and I. Gutman, "Upper bounds for Zagreb indices of connected graphs," *MATCH Commun. Math. Comput. Chem*, vol. 55, pp. 439–446, 2006.

[98] S. Zhang and H. Zhang, "Unicyclic graphs with the first three smallest and largest first general Zagreb index," *MATCH Commun. Math. Comput. Chem*, vol. 55, no. 20, p. 06, 2006.

[99] N. De, "Some bounds of reformulated Zagreb indices," *Appl. Math. Sci*, vol. 6, no. 101, pp. 5005–5012, 2012.

[100] A. Ghalavand and A. R. Ashrafi, "Extremal trees with respect to the first and second reformulated Zagreb index," *Malaya Journal of Matematik (MJM)*, vol. 5, no. 3, 2017, pp. 524–530, 2017.

[101] A. Ilić and B. Zhou, "On reformulated Zagreb indices," *Discrete Applied Mathematics*, vol. 160, no. 3, pp. 204–209, 2012.

[102] S. Ji, X. Li, and B. Huo, "On reformulated Zagreb indices with respect to acyclic, unicyclic and bicyclic graphs," *MATCH Commun. Math. Comput. Chem*, vol. 72, no. 3, pp. 723–732, 2014.

[103] S. Ji, Y. Qu, and X. Li, "The reformulated Zagreb indices of tricyclic graphs," *Applied Mathematics and Computation*, vol. 268, pp. 590–595, 2015.

[104] G. Su, L. Xiong, L. Xu, and B. Ma, "On the maximum and minimum first reformulated Zagreb index of graphs with connectivity at most k," *Filomat*, vol. 25, no. 4, pp. 75–83, 2011.

[105] K. C. Das, M. M. Matejic, E. I. Milovanovic, and I. Z. Milovanovic, "Bounds for symmetric division deg index of graphs," *Filomat*, vol. 33, no. 3, pp. 683–698, 2019.

[106] J. L. Palacios, "New upper bounds for the symmetric division deg index of graphs," *Discrete Math. Lett.*, vol. 2, pp. 52–56, 2019.

[107] B. Furtula, K. Ch. Das, and I. Gutman, "Comparative analysis of symmetric division deg index as potentially useful molecular descriptor," *International Journal of Quantum Chemistry*, vol. 118, no. 17, p. e25659, 2018.

[108] H. Hosoya, "On some counting polynomials in chemistry," *Discrete Applied Mathematics*, vol. 19, no. 1-3, pp. 239–257, 1988.

[109] H. Hosoya, "Topological index. a newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons," *Bulletin of the Chemical Society of Japan*, vol. 44, no. 9, pp. 2332–2339, 1971.

[110] G. G. Cash, "Relationship between the Hosoya polynomial and the hyper-Wiener index," *Applied Mathematics Letters*, vol. 15, no. 7, pp. 893–895, 2002.

[111] E. Deutsch and S. Klavžar, "M-polynomial and degree-based topological indices," *Iranian Journal of Mathematical Chemistry*, vol. 6, pp. 93–102, 2015.

[112] E. Deutsch and S. Klavžar, "M-polynomial revisited: Bethe cacti and an extension of Gutman's approach," *Journal of Applied Mathematics and Computing*, vol. 60, no. 1-2, pp. 253–264, 2019.

[113] Y. C. Kwun, M. Munir, W. Nazeer, S. Rafique, and S. M. Kang, "M-polynomials and topological indices of V-Phenylenic Nanotubes and Nanotori," *Scientific reports*, vol. 7, no. 1, p. 8756, 2017.

[114] M. Munir, W. Nazeer, S. Rafique, and S. Kang, "M-polynomial and degree-based topological indices of polyhex nanotubes," *Symmetry*, vol. 8, no. 12, p. 149, 2016.

[115] M. Rezaei, W. Gao, M. K. Siddiqui, and M. R. Farahani, "Computing hyper-Zagreb index and M-polynomials of Titania nanotubes," *Sigma*, vol. 35, no. 4, pp. 707–714, 2017.

[116] P. Thayamathy, P. Elango, and M. Koneswaran, "M-polynomial and degree based topological indices for Silicon Oxide," *International Research Journal of Pure and Applied Chemistry*, pp. 1–9, 2018.

[117] Y.-J. Ge, J.-B. Liu, M. Younas, M. Yousaf, and W. Nazeer, "Analysis of and nanotubes via topological indices," *Journal of Nanomaterials*, vol. 2019, 2019.

[118] J.-B. Liu, M. Younas, M. Habib, M. Yousaf, and W. Nazeer, "M-polynomials and degree-based topological indices of VC5C7[p, q] and HC5C7[p, q] nanotubes," *IEEE Access*, vol. 7, pp. 41125–41132, 2019.

[119] I. Gutman, A. Ghalavand, T. Dehghan-Zadeh, and A. R. Ashrafi, "Graphs with smallest forgotten index," *Iranian Journal of Mathematical Chemistry*, vol. 8, no. 3, pp. 259–273, 2017.

[120] A. Ghalavand and A. R. Ashrafi, "On forgotten coindex of chemical graphs," *MATCH Commun. Math. Comput. Chem*, vol. 83, pp. 221–232, 2020.

[121] H. Deng, "A unified approach to the extremal Zagreb indices for trees, unicyclic graphs and bicyclic graphs," *MATCH Commun. Math. Comput. Chem*, vol. 57, no. 3, pp. 597–616, 2007.

[122] I. Gutman and O. E. Polansky, *Mathematical concepts in organic chemistry*. Springer Science & Business Media, 2012.

[123] T. Hou, K. Xia, W. Zhang, and X. Xu, "ADME evaluation in drug discovery. 4. Prediction of aqueous solubility based on atom contribution approach," *Journal of chemical information and computer sciences*, vol. 44, no. 1, pp. 266–275, 2004.

[124] S. Amézqueta, X. Subirats, E. Fuguet, M. Rosés, and C. Ràfols, "Octanol-water partition constant," in *Liquid-Phase Extraction* (C. F. Poole, ed.), Handbooks in Separation Science, pp. 183–208, Elsevier, 2020.

[125] S. Hayat and M. Imran, "Computation of certain topological indices of nanotubes covered by C5 and C7," *Journal of Computational and Theoretical Nanoscience*, vol. 12, no. 4, pp. 533–541, 2015.

[126] P. Gramatica, N. Navas, and R. Todeschini, "3d-modelling and prediction by WHIM descriptors. part 9. Chromatographic relative retention time and physico-chemical properties of polychlorinated biphenyls (PCBs)," *Chemometrics and intelligent laboratory systems*, vol. 40, no. 1, pp. 53–63, 1998.

[127] M. Kociak, A. Y. Kasumov, S. Guéron, B. Reulet, I. Khodos, Y. B. Gorbatov, V. Volkov, L. Vaccarini, and H. Bouchiat, "Superconductivity in ropes of single-walled carbon nanotubes," *Physical Review Letters*, vol. 86, no. 11, p. 2416, 2001.

[128] R. H. Baughman, A. A. Zakhidov, and W. A. De Heer, "Carbon nanotubes–the route toward applications," *science*, vol. 297, no. 5582, pp. 787–792, 2002.

[129] M. R. Farahani, "First and second Zagreb polynomials of VC5C7 [p, q] and HC5C7 [p, q] nanotubes," *International Letters of Chemistry, Physics and Astronomy*, vol. 12, 2014.

[130] S. Karunakaran and L. Selvaganesh, "A novel graph matrix representation: Sequence of neighbourhood matrices with an application," *SN Applied Sciences*, vol. 2, no. 5, pp. 1–13, 2020.

[131] E. V. Konstantinova, "The discrimination ability of some topological and information distance indices for graphs of unbranched hexagonal systems," *Journal of chemical information and computer sciences*, vol. 36, no. 1, pp. 54–57, 1996.

[132] S. Mondal, A. Dey, N. De, and A. Pal, "QSPR analysis of some novel neighbourhood degree-based topological descriptors," *Complex & Intelligent Systems*, vol. 7, no. 2, pp. 977–996, 2021.

List of Research Publications

[1] ***Abhay Rajpoot, and Lavanya Selvaganesh.*** "Bounds of the Symmetric Division Deg Index for Trees and Unicyclic Graphs with A Perfect Matching." ***Iranian Journal of Mathematical Chemistry*** (2020) **11(3)**: 141-159. (ESCI, SCOPUS)

[2] ***Abhay Rajpoot, and Lavanya Selvaganesh.*** "Extension of m-polynomial and degree based topological indices for nanotube." ***TWMS Journal of Applied and Engineering Mathematics*** (2021) **11**: 268-279. (ESCI, SCOPUS)

[3] ***Abhay Rajpoot, and Lavanya Selvaganesh.*** "Bounds and Extremal graphs of Second Reformulated Index For Graphs With Cyclomatic Number At Most Three." ***Kuwait Journal of Science*** (2022) **49(1)**: 1-21. (SCIE)

[4] ***Abhay Rajpoot, and Lavanya Selvaganesh.*** "Study of bounds and Extremal Graphs of Symmetric Division Degree Index for Bicyclic graphs with Perfect Matching.", ***Iranian Journal of Mathematical Chemistry*** (2022) **13(2)**: 145-165. (ESCI, SCOPUS)

[5] ***Abhay Rajpoot, and Lavanya Selvaganesh.*** "Predictive Ability of Physicochemical Properties of PCB molecules using Symmetric Division Degree Index." (communicated), 2022

[6] ***Abhay Rajpoot, and Lavanya Selvaganesh.*** "Potential Application of Newly Proposed AL indices as Molecular Descriptors." (communicated), 2022