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Layer matrices and distance property descriptors

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Abstract

Several topological indices-numerical descriptors encoding topological attributes of a molecular graph have been used both in graph discriminating analysis and correlating studies for modeling a variety of physico-chemical properties and biological activities. However, only few software packages, viz., CODESSA, MOLCONN Z, DRAGON, TOSS MODE and POLLY, are available for calculating topological indices. These incorporate correlating analysis statistics, as well. The TOPOCLUJ software package is designed to calculate topological descriptors from topological matrices and/or polynomials. Several weighting schemes including group electronegativity, group mass and partial charges are proposed. Topological indices derived from the matrices like adjacency, connectivity, distance, detour, distance-path, detour-path, Cluj, their reciprocal matrices, walk-matrices, walk-operated matrices, layer- and shell-matrices have been successfully used in correlating studies and graph discriminating analysis during the last decade. Several novel topological matrices, like distance-path, Cluj (with its variants), layer-matrices, walk matrix, walk (triple matrix) operator, characteristic and "property" polynomials, and the corresponding topological descriptors may be calculated by the TOPOCLUJ software package.

References (53)

1. Skorobogatov, V.A., Dobrynin, A.A.
(1988) *MATCH - Commun Math Comput Chem*, 23 p. 105 Cited 12 times

2. Diudea, M.V., Minailiuc, O.M., Balaban, A.T.
(1991) *J Comput Chem*, 12 p. 527 Cited 11 times
View at Publisher

3. Dobrynin, A.A.
(1993) *J Math Chem*, 14 p. 175 Cited 3 times
View at Publisher

4. Yang, Y., Lin, J., Wang, C.
(2002) *J Graph Theory*, 39 p. 219

5. Hu, C.Y., Xu, L.
(1996) *J Chem Inf Comput Sci*, 36 p. 82 Cited 26 times
Abstract + Refs View at Publisher

6. Bonchev, D., Mekanyan, O., Balaban, A.T.
(1989) *J Chem Inf Comput Sci*, 29 p. 91 Cited 7 times
View at Publisher

7. Halberstam, F.Y., Quintas, L.V.

(1982) *Distance and Path Degree Sequences for Cubic Graphs*, Cited 4 times
Pace Univ. New York

8. Randić, M., Woodworth, W.L., Graovac, A.
(1983) *Int J Quantum Chem*, 24 p. 435 Cited 11 times
View at Publisher

9. Diudea, M.V., Gutman, I., Jäntschi, L.
(2001) *Molecular Topology*, Cited 13 times
NOVA, Huntington, New York

10. Diudea, M.V., Ursu, O.
(2002) *TOPOCLUJ*, Cited 2 times
Copyright Babes-Bolyai Univ. Cluj

11. Diudea, M.V.
(1994) *J Chem Inf Comput Sci*, 34 p. 1064 Cited 22 times
Abstract + Refs View at Publisher

12. Diudea, M.V., Topan, M.I., Graovac, A.
(1994) *J Chem Inf Comput Sci*, 34 p. 1072 Cited 16 times
Abstract + Refs View at Publisher

13. Diudea, M.V.
MATCH - Commun Math Comput Chem (MATCH),
In press

14. Wiener, H.
(1947) *J Am Chem Soc*, 69 p. 17 Cited 736 times
View at Publisher

15. Diudea, M.V., Gutman, I.
(1998) *Croat Chem Acta*, 71 p. 21 Cited 56 times
Abstract + Refs

16. Diudea, M.V.
(1996) *J Chem Inf Comput Sci*, 36 p. 833 Cited 41 times
Abstract + Refs View at Publisher

17. Ivanciuc, O., Balaban, T.S., Balaban, A.T.
(1993) *J Math Chem*, 12 p. 309 Cited 77 times
View at Publisher

18. Plavšić, D., Nikolić, S., Trinajstić, N., Mihalić, Z.
(1993) *J Math Chem*, 12 p. 235 Cited 71 times
View at Publisher

19. Diudea, M.V.
(1997) *J Chem Inf Comput Sci*, 37 p. 292 Cited 41 times
Abstract + Refs View at Publisher

20. Estrada, E., Rodriguez, L., Gutierrez, A.
(1997) *MATCH - Commun Math Comput Chem*, 35 p. 145 Cited 17 times
Abstract + Refs

21. Kier, L.B., Hall, L.H.
(1999) *Molecular Structure Description: The Electrotopological State*, Cited 210 times
Academic Press, San Diego

22. Diudea, M.V.
(1999) *Croat Chem Acta*, 72 p. 835 Cited 8 times
Abstract + Refs

23. Schultz, H.P.
(1989) *J Chem Inf Comput Sci*, 29 p. 227 Cited 92 times
Abstract + Refs View at Publisher

24. Ivanciuc, O.
(2000) *Rev Roum Chem*, 45 p. 587 Cited 13 times
Abstract + Refs

25. Dobrynin, A., Kochetova, A.A.
(1994) *J. Chem Inf Comput Sci*, 34 p. 1082 Cited 14 times

Abstract + Refs View at Publisher

26. Estrada, E., Rodriguez, L.
(1997) *MATCH - Commun Math Comput Chem*, 35 p. 157 Cited 12 times
Abstract + Refs

27. Diudea, M.V.
(1996) *J Chem Inf Comput Sci*, 36 p. 535 Cited 46 times
Abstract + Refs View at Publisher

28. Harary, F.
(1969) *Graph Theory*, Cited 1264 times
Addison-Wesley, Reading, MA

29. Klein, D.J., Lukovits, I., Gutman, I.
(1995) *J Chem Inf Comput Sci*, 35 p. 50 Cited 72 times
Abstract + Refs View at Publisher

30. Diudea, M.V., Randić, M.
(1997) *J Chem Inf Comput Sci*, 37 p. 1095 Cited 5 times
Abstract + Refs View at Publisher

31. Horn, R.A., Johnson, C.R.
(1985) *Matrix Analysis*, Cited 2964 times
Cambridge Univ. Press, Cambridge

32. Randić, M., Guo, X., Oxley, T., Krishnapriyan, H.
(1993) *J Chem Inf Comput Sci*, 33 p. 700 Cited 7 times

33. Randić, M., Guo, X., Oxley, T., Krishnapriyan, H., Naylor, L.
(1994) *J Chem Inf Comput Sci*, 34 p. 361 Cited 74 times
Abstract + Refs View at Publisher

34. Diudea, M.V.
(1997) *J Chem Inf Comput Sci*, 37 p. 300 Cited 40 times
Abstract + Refs View at Publisher

35. Diudea, M.V.
(1997) *MATCH - Commun Math Comput Chem*, 35 p. 169 Cited 23 times
Abstract + Refs

36. Diudea, M.V., Parv, B., Gutman, I.
(1997) *J Chem Inf Comput Sci*, 37 p. 1101 Cited 16 times
Abstract + Refs View at Publisher

37. Gutman, I., Diudea, M.V.
(1998) *J Serb Chem Soc*, 63 p. 497 Cited 2 times
Abstract + Refs

38. Diudea, M.V., Katona, G., Lukovits, I., Trinajstić, N.
(1998) *Croat Chem Acta*, 71 p. 459 Cited 4 times
Abstract + Refs

39. Jäntschi, L., Katona, G., Diudea, M.V.
(2000) *MATCH - Commun Math Comput Chem*, 41 p. 151 Cited 5 times
Abstract + Refs

40. Diudea, M.V., Ivanciuc, O.
(1995) *Molecular Topology*, Cited 45 times
COMPREX, Cluj

41. Dwyes, P.S.
(1951) *Linear Computations*, Cited 11 times
Wiley, New York

42. Fadeev, D.K., Sominskii, I.S.
(1965) *Problems in Higher Algebra*, Cited 7 times
Freeman, San Francisco

43. Hosoya, H.
(1971) *Bull Chem Soc Japan*, 44 p. 2332 Cited 340 times

44. Hosoya, H.
(1988) *Discrete Appl Math*, 19 p. 239 Cited 45 times
Abstract + Refs View at Publisher

45. Ivanciuc, O.
(2001) *Rev Roum Chem*, 46 p. 129 Cited 3 times
Abstract + Refs

46. Cvetković, D.M., Gutman, I.
(1977) *Croat Chem Acta*, 49 p. 115 Cited 32 times

47. Diudea, M.V., Ivanciuć, O., Nikolić, S., Trinajstić, N.
(1997) *MATCH - Commun Math Comput Chem*, 35 p. 41 Cited 39 times
Abstract + Refs

48. Randić, M.
(2001) *J Chem Inf Comput Sci*, 41 p. 627 Cited 12 times
Abstract + Refs View at Publisher

49. Katritzky, A.R., Lobanov, V.S., Karelson, M.
(1996) *CODESSA Reference Manual*, Cited 61 times
Ver. 2.0, Univ. Florida

50.
MOLCONN-Z,
Hall associates consulting, Quincy, MA, 02170, USA

51. Todeschini, R., Consonni, V.
(2000) *Handbook of Molecular Descriptors*, Cited 372 times
Wiley-VCH, Dragon 1.1 software package

52. Gutierrez, Y., Estrada, E., Rodriguez, L., Munoz, I.
(1995) *TOSS_MODE, Ver. 2.5 for Window*,
Central Univ. Las Villas, Santa Clara, Cuba

53. Basak, S.C., Harris, D.K., Magnuson, V.R.
(1988) *POLLY 2.3*, Cited 20 times
Copyright Univ. Minnesota

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