

Quick Search [Search History](#) [Results list](#) **1 of 1**

[Letters in Drug Design and Discovery](#)










Volume 2, Issue 8, December 2005, Pages 606-624

DOI: 10.2174/157018005774717334

Document Type: Review

[Output](#) [Add to list](#)[View references](#) (176)[View at Publisher](#)

Szeged index - Applications for drug modeling

[Khadikar, P.V.](#)^a  , [Karmarkar, S.](#)^a , [Agrawal, V.K.](#)^b , [Singh, J.](#)^b ,
[Shrivastava, A.](#)^c , [Lukovits, I.](#)^d , [Diudea, M.V.](#)^e  

^a Research Division, Laxmi Fumigation and Pest Control, Pvt. Ltd., 3, Khatipura, Indore 452 007, India

^b Department of Chemistry, A.P.S. University, Rewa, 486 003, India

^c Department of Chemistry, Holkar Model and Autonomous College, Indore 452 001, India

^d Central Research Institute for Chemistry, Hungarian Academy of Sciences, P.O. Box 17, H-1525, Budapest, Hungary

[Basic Format](#) [Extended Format](#)

Cited By since 1996

This article has been cited **3** times in

Scopus:
(Showing the 2 most recent)

[Singh, J.](#),
[Singh, S.](#),
[Meer, S.](#)

QSPR correlations

^e Faculty of Chemistry and Chemical Engineering, Babes-Bolyai University, 3400 Cluj, Romania

Abstract

In this review we describe various applications of Szeged (Sz) index for modeling physicochemical properties as well as physiological activities of organic compounds acting as drugs or possess pharmacological activity. © 2005 Bentham Science Publishers Ltd.

Author Keywords

Biological activity; Drug design; Multiple regression analysis; Physicochemical properties; QSAR; QSPR; QSTR; Szeged index

References (176)

↙    Output Select: Page

1. Wiener, H.
Structural determination of paraffin boiling points
(1947) *Journal of the American Chemical Society*, 69 (1), pp. 17-20. [Cited 884 times](#).

[Abstract + Refs](#) [View at Publisher](#)

**of half-wave
reduction
potentials of
cata-
condensed
benzenoid
hydrocarbons**

(2006) *Arkivoc*

[Abstract + Refs](#)

. [Agrawal, V.K.](#)
, [Singh, J.](#) ,
[Louis, B.](#)

**The topology
of molecule
and its
lipophilicity**
(2006) *Current
Computer-
Aided Drug
Design*

2. □ Gutman, I.
(1994) *Graph Theory Notes New York*, 27, pp. 9-15. [Cited 133 times](#).
3. □ Dobrynin, A., Gutman, I.
(1994) *Publ. Inst. Math. (Belgrade)*, 56, pp. 18-22. [Cited 30 times](#).
4. □ Dobrynin, A., Gutman, I.
(1995) *Graph Theory Notes New York*, 28, pp. 21-23. [Cited 26 times](#).
5. □ Dobrynin, A., Gutman, I., Domotor, G.
(1995) *Appl. Maths. Lett.*, 8, pp. 57-62. [Cited 29 times](#).

[View at Publisher](#)

6. □ Khadikar, P.V., Deshpande, N.V., Kale, P.P., Dobrynin, A., Gutman, I., Dömötör, G.
The Szeged index and an analogy with the Wiener index
(1995) *Journal of Chemical Information and Computer Sciences*, 35 (3), pp. 547-550. [Cited 120 times](#).

[Abstract + Refs](#) [View at Publisher](#)

7. □ Gutman, I., Klavžar, S.
An algorithm for the calculation of the Szeged index of

[Abstract + Refs](#)

[View details of all 3 citations](#)

Inform me when this document is cited in Scopus:

- [E-mail Alert](#)
-  [RSS](#)

Find related documents

In Scopus based on

-  [references](#)
-  [authors](#)
-  [keywords](#)

On the Web based on

benzenoid hydrocarbons

(1995) *Journal of Chemical Information and Computer Sciences*, 35 (6), pp. 1011-1014. [Cited 34 times](#).

[Abstract + Refs](#) [View at Publisher](#)

[title](#)

[authors](#)

[keywords](#)

8. □ Gutman, I., Khadikar, P.V., Rajput, P.V., Karmarkar, S. (1995) *J. Serb. Chem. Soc.*, 60, pp. 759-764. [Cited 22 times](#).

9. □ Klavžar, S., Rajapakse, A., Gutman, I.

The Szeged and the Wiener index of graphs

(1996) *Applied Mathematics Letters*, 9 (5), pp. 45-49. [Cited 20 times](#).

doi: 10.1016/0893-9659(96)00071-7

[Abstract + Refs](#) [View at Publisher](#)

10. □ Žerovnik, J.

Computing the Szeged Index

(1996) *Croatica Chemica Acta*, 69 (3), pp. 837-843. [Cited 11 times](#).

[Abstract + Refs](#)

11. □ Dobrynin, A.A., Gutman, I.

On the Szeged Index of Unbranched Catacondensed Benzenoid Molecules

(1996) *Croatica Chemica Acta*, 69 (3), pp. 845-856. [Cited 15 times.](#)

[Abstract + Refs](#)

12. □ Gutman, I., Klavžar, S.
A method for calculating Wiener numbers of benzenoid hydrocarbons
(1996) *ACH - Models in Chemistry*, 133 (4), pp. 389-399. [Cited 31 times.](#)

[Abstract + Refs](#)

13. □ Gutman, I., Dömötör, G., Lam, P.C.B., Shiu, W.C., Popović, L.
Szeged indices of benzenoid hydrocarbons
(1996) *Polycyclic Aromatic Compounds*, 8 (4), pp. 259-270. [Cited 8 times.](#)

[Abstract + Refs](#)

14. □ Khadikar, P.V., Karmarkar, S., Joshi, S., Gutman, I.
Estimation of the protonation constants of salicylhydroxamic acids by means of the Wiener topological index
(1996) *Journal of the Serbian Chemical Society*, 61 (2), pp. 89-95. [Cited 28 times.](#)

[Abstract + Refs](#)

15. □ Gutman, I.
(1996) *Bull. Acad. Serb. Sci. Arts, (C/Math Natut)*, 111, pp. 19-29. [Cited 4 times](#).
16. □ Gutman, I., Popović, L., Pavlović, L.
Elementary edge-cuts in the theory of benzenoid hydrocarbons - An application
(1997) *Match*, 36, pp. 217-229. [Cited 7 times](#).

[Abstract + Refs](#)

17. □ Diudea, M.V., Minailiuc, O.M., Katona, G., Gutman, I.
Szeged matrices and related numbers
(1997) *Match*, 35, pp. 129-143. [Cited 33 times](#).

[Abstract + Refs](#)

18. □ Gutman, I.
Wiener numbers of benzenoid isomers containing a linear polyacene fragment
(1997) *Indian Journal of Chemistry - Section A Inorganic, Physical, Theoretical and Analytical Chemistry*, 36 (8), pp. 644-648. [Cited 5 times](#).

[Abstract + Refs](#)

19. □ Diudea, M.V., Par v, B., Tofan, M.I.

Derived Szeged and Cluj indices

(1997) *Journal of the Serbian Chemical Society*, 62 (3), pp. 267-276. [Cited 27 times](#).

[Abstract + Refs](#)

20. □ Kiss, A.A., Kacso, I.E., Minailiuc, O.M., Diudea, M.V., Nicolice, S., Gutman, I.
(1997) *Studia Univ. Babes-Bolyai (Ser. Chem)*, 42, pp. 183-192. [Cited 2 times](#).

21. □ (2000) *Kragujevac J. Chem.*, 22, pp. 49-58.

22. □ (1997) *Studia Univ Babes-Bolyai, Chemia*, 42, pp. 1-8.

23. □ Gutman, I.

Comparing Wiener numbers of isomeric benzenoid hydrocarbons

(1997) *ACH - Models in Chemistry*, 134 (4), pp. 477-486. [Cited 4 times](#).

[Abstract + Refs](#)

24. □ Lukovits, I.

Szeged Index: Formulas for Fused Bicyclic Graphs

(1997) *Croatica Chemica Acta*, 70 (3), pp. 863-871. [Cited 4 times](#).

[Abstract + Refs](#)

25. □ Dobrynin, A.A.
Graphs Having the Maximal Value of the Szeged Index
(1997) *Croatica Chemica Acta*, 70 (3), pp. 819-825. [Cited 6 times](#).

[Abstract + Refs](#)

26. □ Gutman, I., Klavzar, S.J.
Relations between Wiener numbers of benzenoid hydrocarbons and phenylenes
ACH-Models in Chemistry
Personal communication

27. □ Diudea, M.V., Gutman, I.
Wiener-type topological indices - A jungle guide
Croat. Chem. Acta.
Personal communication

28. □ Diudea, M.V.
Indices of reciprocal properties or Harary indices
(1997) *Journal of Chemical Information and Computer Sciences*, 37 (2), pp. 292-299. [Cited 44 times](#).

[Abstract + Refs](#) [View at Publisher](#)

29. □ Chepoi, V., Klavžar, S.
The Wiener index and the Szeged index of benzenoid

systems in linear time

(1997) *Journal of Chemical Information and Computer Sciences*, 37 (4), pp. 752-755. [Cited 15 times](#).

[Abstract + Refs](#) [View at Publisher](#)

30. □ Gutman, I., Popović, L., Khadikar, P.V., Karmarkar, S., Joshi, S., Mandloi, M.

Relations between Wiener and Szeged indices of monocyclic molecules

(1997) *Match*, 35, pp. 91-103. [Cited 21 times](#).

[Abstract + Refs](#)

31. □ Gutman, I., Khadikar, P.V., Khaddar, T.

Wiener and Szeged indices of benzenoid hydrocarbons containing a linear polyacene fragment

(1997) *Match*, 35, pp. 105-116. [Cited 22 times](#).

[Abstract + Refs](#)

32. □ Dobrynin, A.A., Gutman, I.

Szeged index of some polycyclic bipartite graphs with circuits of different size

(1997) *Match*, 35, pp. 117-128. [Cited 11 times](#).

[Abstract + Refs](#)

33. □ Diudea, M.V.

Cluj matrix invariants

(1997) *Journal of Chemical Information and Computer Sciences*, 37 (2), pp. 300-305. [Cited 42 times](#).

[Abstract + Refs](#) [View at Publisher](#)

34. □ Dobrynin, A.A.

The Szeged index for complements of hexagonal chains

(1997) *Match*, 35, pp. 227-242. [Cited 10 times](#).

[Abstract + Refs](#)

35. □ Dobrynin, A.A., Gutman, I.

(1997) *Elektrotehn Fak (Beograd)*, 8, pp. 106-113. [Cited 4 times](#).

36. □ Karmarkar, S., Karmarkar, S., Joshi, S., Das, A., Khadikar, P.V.

Novel application of Wiener vis-a-vis Szeged indices in predicting polychlorinated biphenyls in the environment

(1997) *Journal of the Serbian Chemical Society*, 62 (3), pp. 227-234. [Cited 13 times](#).

[Abstract + Refs](#)

37. □ Das, A., Dömötör, G., Gutman, I., Joshi, S., Karmarkar,

S., Khaddar, D., Khaddar, T., (...), Shirhatti, A.

A comparative study of the Wiener, Schultz and Szeged indices of cycloalkanes

(1997) *Journal of the Serbian Chemical Society*, 62 (3), pp. 235-239. [Cited 11 times](#).

[Abstract + Refs](#)

38. □ Schirger, I., Diudea, M.V.
(1997) *Studia Univ Babes-Bolyai, Chemia*, 42, pp. 269-280. [Cited 2 times](#).
39. □ Kiss, A.A., Katona, G., Diudea, M.V.
(1997) *Coll. Sci. Papers Fac. Sci. Kragujevac*, 19, pp. 95-107. [Cited 15 times](#).
40. □ Marjanovic, M., Gutman, I.
(1997) *Bull. Acad. Serbe Sci. Arts*, 114, pp. 99-108. [Cited 4 times](#).
41. □ Gutman, I., Dobrynin, A.A.
(1998) *Graph Theory Notes New York*, 34, pp. 37-44. [Cited 21 times](#).
42. □ Diudea, M.V., Gutman, I.
Wiener-Type Topological Indices
(1998) *Croatica Chemica Acta*, 71 (1), pp. 21-25. [Cited 66](#)

[times.](#)

[Abstract + Refs](#) [View at Publisher](#)

43. □ Gutman, I., Klavzar, S.
Relations between Wiener numbers of benzenoid hydrocarbons and phenylenes
(1998) *ACH - Models in Chemistry*, 135 (1-2), pp. 45-55. [Cited 8 times.](#)
- [Abstract + Refs](#)
44. □ Ivanciuc, O., Diudea, M.V., Kartona, G., Schirgei, I., Kiss, A.A., Dobrynin, A.A.
Cluj and Szeged Polynomials
Personal communication
45. □ Minailiuc, O.M., Katona, G., Diudea, M.V., Strunje, M., Graovac, A., Gutman, I.
Szeged Fragmental Indices
(1998) *Croatica Chemica Acta*, 71 (3), pp. 473-488. [Cited 7 times.](#)
- [Abstract + Refs](#) [View at Publisher](#)
46. □ Dobrynin, A.A.
The Szeged Index of Line Graphs
Personal communication

47. □ Žerovnik, J.
Szeged index of symmetric graphs
(1999) *Journal of Chemical Information and Computer Sciences*, 39 (1), pp. 77-80. [Cited 3 times](#).
[Abstract + Refs](#) [View at Publisher](#)
48. □ Enovnik, J.
(2000) *J. Chem. Inf. Comput. Sci.*, 40, pp. 77-80.
49. □ Ivanciuc, O.
Design of topological indices part 17. The Szeged operator as a source of new structural descriptors
Rev. Roum. Chem.
Personal communication
50. □ Agrawal, V.K., Bano, S., Mathur, K.C., Khadikar, P.V.
(1999) *Proc. Nat. Acad. Sci. India*, 69, pp. 145-154. [Cited 5 times](#).
51. □ Agrawal, V.K., Bano, S., Mathur, K.C., Khadikar, P.V., Karmarkar, S.
(1999) *Nat. Acad. Sci. Lett.*, 22, pp. 55-59. [Cited 8 times](#).
52. □ Sachan, S., Bano, S., Agrawal, V.K., Khadikar, P.V., Shrivastava, A.K.
(1999) *Nat. Acad. Sci. Lett.*, 22, pp. 119-124. [Cited 3 times](#).

53. □ Jantschi, L., Muresen, S., Diudea, M.V.
(1999) *Studia Univ. Babeş-Bolyai, Chemia.*, 44, pp. 10-15.
54. □ Khadikar, P.V., Karmarkar, S., Agrawal, V.K., Mandloi, M., Joshi, S.
(2000) *Nat. Acad. Sci. Lett.*, 23, pp. 50-56. [Cited 4 times](#).
55. □ Sharma Karmarkar, S., Thakral, G.B., Khadikar, P.V.
(2000) *Nat. Acad. Sci. Lett.*, 23, pp. 81-85. [Cited 2 times](#).
56. □ Khadikar, P.V., Karmarkar, S., Agrawal, V.K.
(2000) *Nat. Acad. Sci. Lett.*, 23, pp. 165-170. [Cited 16 times](#).
57. □ Agrawal, V.K.
Novel application of Wiener vis-à-vis Szeged indices: Antitubercular activities of quinolones
(2000) *Proceedings of the Indian Academy of Sciences: Chemical Sciences*, 112 (2), pp. 137-146. [Cited 5 times](#).
[Abstract + Refs](#)
58. □ Karmarkar, S., Saxena, A., Verma, R.G., Karmarkar, S., Mathur, K., Mathur, S., Singh, S., (...), Khadikar, P.
Determining environmental behaviour and biological activity of RDX and related compounds
(2000) *Pollution Research*, 19 (3), pp. 337-344. [Cited 5](#)

[times.](#)

[Abstract + Refs](#)

59. □ Agrawal, V.K., Sachan, S., Khadikar, P.V.
Topological potential of zwitterion analogues of cimetidine as H receptor antagonists
(2000) *Polish Journal of Pharmacology*, 52 (1), pp. 39-46. [Cited 9 times.](#)

[Abstract + Refs](#)

60. □ Khadikar, P.V., Kale, P.P., Deshpande, N.V., Agrawal, V.K.
On the Szeged index of monocyclic graphs
(2000) *Journal of the Indian Chemical Society*, 77 (9), pp. 449-452. [Cited 6 times.](#)

[Abstract + Refs](#)

61. □ Mandloi, M., Sikarwar, A., Sapre, N.S., Karmarkar, S., Khadikar, P.V.
A Comparative QSAR Study Using Wiener, Szeged, and Molecular Connectivity Indices
(2000) *Journal of Chemical Information and Computer Sciences*, 40 (1), pp. 57-62. [Cited 21 times.](#)

[Abstract + Refs](#) [View at Publisher](#)

62. □ Karmarkar, S., Joshi, S., Sharma, V., Khadikar, P.

Correlation potential of Wiener vis-a-vis Szeged indices: Anti-inflammatory activities of phenols

(2000) *Journal of the Indian Chemical Society*, 77 (9), pp. 433-437. [Cited 5 times](#).

[Abstract + Refs](#)

63. □ Joshi, S., Karmarkar, S., Khadikar, P.V.
(2000) *Sci. & Cult.*, 66, pp. 268-290.

64. □ Mandloi, M., Agrawal, V.K., Mathur, K.C., Karmarkar, S., Khadikar, P.V.

QSAR analysis of indolealkylamine receptor binding using Szeged index

(2000) *Acta Pharmaceutica*, 50 (4), pp. 303-313. [Cited 7 times](#).

[Abstract + Refs](#)

65. □ Agrawal, V.K., Sachan, S., Khadikar, P.V.

QSAR studies on antihistaminic activity of some thiazolidine-4-ones

(2000) *Acta Pharmaceutica*, 50 (4), pp. 281-290. [Cited 8 times](#).

[Abstract + Refs](#)

66. □ Simic, S., Gutman, I., Baltic, V.

(2000) *Math Slovaca*, 50, pp. 1-15.

67. □ Mathur, K.C., Khadikar, P.V., Chauhan, U.K., Shrivastava, R.
(2001) *Res. J. Chem. Environ.*, 5, pp. 68-70. [Cited 3 times](#).

68. □ Mathur, K.C., Chauhan, U.K., Shrivastava, R., Khadikar, P.V.
(2001) *Orient. J. Chem.*, 7, pp. 253-256. [Cited 2 times](#).

69. □ Sapre, N.S., Sikarwar, A., Khadikar, P.V.

A QSPR study on salicylhydroxamic acids using Szeged index (Sz)

(2001) *Oxidation Communications*, 24 (1), pp. 38-47. [Cited 2 times](#).

[Abstract + Refs](#)

70. □ Agrawal, V.K., Bano, S., Khadikar, P.V.

QSAR modelling of antihypertensive thiadiazoles

(2001) *Oxidation Communications*, 24 (1), pp. 21-27. [Cited 2 times](#).

[Abstract + Refs](#)

71. □ Khadikar, P., Kale, P., Deshpande, N., Karmarkar, S., Agrawal, V.

Szeged indices of hexagonal chains

(2001) *Match*, 43, pp. 7-15. [Cited 20 times](#).

[Abstract + Refs](#)

72. □ Agrawal, V.K., Srivastava, R., Khadikar, P.V.
QSAR studies on some antimalarial sulfonamides.
(2001) *Bioorganic & medicinal chemistry*, 9 (12), pp. 3287-3293. [Cited 23 times](#).
doi: 10.1016/S0968-0896(01)00241-3
[Abstract + Refs](#) [View at Publisher](#)
73. □ Agrawal, V.K., Khadikar, P.V.
QSAR prediction of toxicity of nitrobenzenes
(2001) *Bioorganic and Medicinal Chemistry*, 9 (11), pp. 3035-3040. [Cited 28 times](#).
doi: 10.1016/S0968-0896(01)00211-5
[Abstract + Refs](#) [View at Publisher](#)
74. □ Khadikar, P.V., Karmarkar, S., Agrawal, V.K.
A Novel PI Index and its Applications to QSPR/QSAR Studies
(2001) *Journal of Chemical Information and Computer Sciences*, 41 (4), pp. 934-949. [Cited 62 times](#).
doi: 10.1021/ci0003092
[Abstract + Refs](#) [View at Publisher](#)
75. □ Agrawal, V.K., Karmarkar, S., Khadikar, P.V.
QSAR study on binding affinity of PATs (rodenticides)

to the [3H]-mepyramine-labelled H1 receptor in rat and guinea pig brain.

(2001) *SAR and QSAR in environmental research*, 12 (6), pp. 529-545. [Cited 6 times](#).

[Abstract + Refs](#)

76. □ Karmarkar, S., Khadikar, P.V., Mandloi, M., Joshi, S., Agrawal, V.K.

Topological estimation of proton-ligand formation constants: A multivariate analysis

(2001) *Indian Journal of Chemistry - Section A Inorganic, Physical, Theoretical and Analytical Chemistry*, 40 (1), pp. 12-22. [Cited 11 times](#).

[Abstract + Refs](#)

77. □ Katona, G., Turcu, G., Kiss, A.A., Minailiuc, O.M., Diudea, M.V.

(2001) *Rev. Roumaine Chim.*, 46, pp. 137-151.

78. □ Kiss, A.A., Turcu, G., Diudea, M.V.

(2001) *Studia Univ Babeş-Bolyai, Chemia*, 45, pp. 99-106. [Cited 2 times](#).

79. □ Agrawal, V.K., Khadikar, P.V.

Modelling of anti-HIV-1 drugs: Acyclouridine

derivatives

(2002) *Oxidation Communications*, 25 (4), pp. 481-492.

[Abstract + Refs](#)

80. □ Mandloi, M., Agrawal, V.K., Mathur, K.C., Karmarkar, S., Khadikar, P.V.

Estimation of antihypertensive activity of 2-aryl-imino-imidazolidines using Szeged index

(2002) *Oxidation Communications*, 25 (2), pp. 193-202.

[Abstract + Refs](#)

81. □ Khadikar, P.V., Bajaj, A.V., Mandloi, D.

Prediction of C nuclear magnetic resonance chemical shifts (ΣC) in alkanes and cycloalkanes

(2002) *Indian Journal of Chemistry - Section A Inorganic, Physical, Theoretical and Analytical Chemistry*, 41 (10), pp. 2065-2067. [Cited 13 times](#).

[Abstract + Refs](#)

82. □ Agrawal, V.K., Khadikar, P.V.

(2002) *Bulg. Chem. Commun.*, 34, pp. 1-6.

83. □ Agrawal, V.K., Khadikar, P.V.

(2002) *Bulg. Chem. Ind.*, 73, pp. 11-16. [Cited 2 times](#).

84. □ Mandloi, M., Agrawal, V.K., Mathur, K.C., Karmarkar,

S., Khadikar, P.V.

(2002) *Bulg. Chem. Ind.*, 73, pp. 5-10.

85. □ Agrawal, V.K., Singh, J., Khadikar, P.V.

On the topological evidences for modelling lipophilicity

(2002) *Bioorganic and Medicinal Chemistry*, 10 (12), pp.

3981-3996. [Cited 15 times](#).

doi: 10.1016/S0968-0896(02)00299-7

[Abstract + Refs](#) [View at Publisher](#)

86. □ Agrawal, V.K., Sharma, R., Khadikar, P.V.

Quantitative structure-activity relationship studies on 5-phenyl-3-ureido-1,5-benzodiazepine as cholecystinin-A receptor antagonists

(2002) *Bioorganic and Medicinal Chemistry*, 10 (11), pp.

3571-3581. [Cited 8 times](#).

doi: 10.1016/S0968-0896(02)00167-0

[Abstract + Refs](#) [View at Publisher](#)

87. □ Khadikar, P.V., Agrawal, V.K., Karmarkar, S.

Prediction of lipophilicity of polyacenes using quantitative structure-activity relationships

(2002) *Bioorganic and Medicinal Chemistry*, 10 (11), pp.

3499-3507. [Cited 20 times](#).

doi: 10.1016/S0968-0896(02)00226-2

[Abstract + Refs](#) [View at Publisher](#)

88. □ Khadikar, P.V., Karmarkar, S., Singh, S., Shrivastava, A.
Use of the PI index in predicting toxicity of nitrobenzene derivatives

(2002) *Bioorganic and Medicinal Chemistry*, 10 (10), pp. 3163-3170. [Cited 14 times](#).

doi: 10.1016/S0968-0896(02)00211-0

[Abstract + Refs](#) [View at Publisher](#)

89. □ Agrawal, V.K., Sharma, R., Khadikar, P.V.
QSAR studies on carbonic anhydrase inhibitors: A case of ureido and thioureido derivatives of aromatic/heterocyclic sulfonamides

(2002) *Bioorganic and Medicinal Chemistry*, 10 (9), pp. 2993-2999. [Cited 22 times](#).

doi: 10.1016/S0968-0896(02)00123-2

[Abstract + Refs](#) [View at Publisher](#)

90. □ Agrawal, V.K., Sohgaurya, R., Khadikar, P.V.
QSAR studies on biological activity of piritrexim analogues against pc DHFR

(2002) *Bioorganic and Medicinal Chemistry*, 10 (9), pp.

2919-2926. [Cited 2 times](#).

doi: 10.1016/S0968-0896(02)00159-1

[Abstract + Refs](#) [View at Publisher](#)

91. □ Khadikar, P.V., Pathre, S.V., Shrivastava, A.
Structural assignment of 2,6- and 2,7-disubstituted naphthalenes and prediction of C nuclear magnetic resonance chemical shifts: Applications of topology and two-dimensional NMR spectroscopy
(2002) *Bioorganic and Medicinal Chemistry Letters*, 12 (19), pp. 2673-2680. [Cited 8 times](#).
doi: 10.1016/S0960-894X(02)00556-5

[Abstract + Refs](#) [View at Publisher](#)

92. □ Khadikar, P.V., Phadnis, A., Shrivastava, A.
QSAR study on toxicity to aqueous organisms using the PI index
(2002) *Bioorganic and Medicinal Chemistry*, 10 (4), pp. 1181-1188. [Cited 18 times](#).
doi: 10.1016/S0968-0896(01)00375-3

[Abstract + Refs](#) [View at Publisher](#)

93. □ Agrawal, V.K., Sharma, R., Khadikar, P.V.
QSAR studies on antimalarial substituted phenyl

analogues and their N-oxides

(2002) *Bioorganic and Medicinal Chemistry*, 10 (5), pp. 1361-1366. [Cited 5 times](#).

doi: 10.1016/S0968-0896(01)00399-6

[Abstract + Refs](#) [View at Publisher](#)

94. □ Agrawal, V.K., Karmarkar, S., Khadikar, P.V., Shrivastava, S., Lukovits, I.

Use of distance-based topological indices in modeling antihypertensive activity: Case of 2-aryl-imino-imidazolidines

(2003) *Indian Journal of Chemistry - Section A Inorganic, Physical, Theoretical and Analytical Chemistry*, 42 (6), pp. 1426-1435. [Cited 6 times](#).

[Abstract + Refs](#)

95. □ Khadikar, P.V., Lukovits, I., Agrawal, V.K., Shrivastava, S., Jaiswal, M., Gutman, I., Karmarkar, S., (...), Shrivastava, A.

Equalized electronegativity and topological indices: Application for modeling toxicity of nitrobenzene derivatives

(2003) *Indian Journal of Chemistry - Section A Inorganic, Physical, Theoretical and Analytical Chemistry*, 42 (6), pp.

1436-1441. [Cited 14 times](#).

[Abstract + Refs](#)

96. □ Mathur, K.C., Gupta, S., Khadikar, P.V.
Topological modelling of analgesia
(2003) *Bioorganic and Medicinal Chemistry*, 11 (8), pp.
1915-1928. [Cited 6 times](#).
doi: 10.1016/S0968-0896(02)00560-6

[Abstract + Refs](#) [View at Publisher](#)

97. □ Agrawal, V.K., Khadikar, P.V.
**Qsar study on antihypertensive activity of a series of
alkyl N-[diphenylalkyl]aminoalkyl-4-aryl-1,4-dihydro-
2,6- dimethylpyridine-3,5-dicarboxylates**
(2003) *Oxidation Communications*, 26 (1), pp. 1-8.

[Abstract + Refs](#)

98. □ Agrawal, V.K., Bano, S., Khadikar, P.V.
**Topological approach to quantifying molecular
lipophilicity of heterogeneous set of organic
compounds**
(2003) *Bioorganic and Medicinal Chemistry*, 11 (18), pp.
4039-4047. [Cited 9 times](#).
doi: 10.1016/S0968-0896(03)00370-5

[Abstract + Refs](#) [View at Publisher](#)

99. □ Agrawal, V.K., Chaturvedi, S., Abraham, M.H., Khadikar, P.V.
QSAR study on tadpole narcosis
(2003) *Bioorganic and Medicinal Chemistry*, 11 (20), pp. 4523-4533. [Cited 4 times](#).
doi: 10.1016/S0968-0896(03)00446-2

[Abstract + Refs](#) [View at Publisher](#)

100. □ Khadikar, P., Mandloi, M., Shrivastava, A., Phadnis, A.
Topological estimation of characteristic vibration of carbonyl group
(2003) *Oxidation Communications*, 26 (2), pp. 161-167. [Cited 3 times](#).

[Abstract + Refs](#)

101. □ Khadikar, P.V., Singh, S., Mandloi, D., Joshi, S., Bajaj, A.V.
QSAR study on bioconcentration factor (BCF) of polyhalogenated biphenyls using the PI index
(2003) *Bioorganic and Medicinal Chemistry*, 11 (23), pp. 5045-5050. [Cited 7 times](#).
doi: 10.1016/j.bmc.2003.08.028

[Abstract + Refs](#) [View at Publisher](#)

102. □ Agrawal, V.K., Srivastava, S., Khadikar, P.V., Supuran, C.T.

Quantitative structure-activity relationship study on sulfanilamide schiff's bases: Carbonic anhydrase (CA) inhibitors

(2003) *Bioorganic and Medicinal Chemistry*, 11 (24), pp.

5353-5362. [Cited 16 times](#).

doi: 10.1016/j.bmc.2003.09.037

[Abstract + Refs](#) [View at Publisher](#)

103. □ Adhikari, S.K., Sinha, D.K., Mukherjee, D.C.

On the study of Szeged index and Wiener index for monocyclic graphs from geodesic topological matrices

(2003) *Journal of the Indian Chemical Society*, 80 (5), pp.

597-599.

[Abstract + Refs](#)

104. □ Agrawal, V.K., Bano, S., Khadikar, P.V.

QSAR study on 5-lipoxygenase inhibitors using distance-Based topological indices

(2003) *Bioorganic and Medicinal Chemistry*, 11 (24), pp.

5519-5527. [Cited 3 times](#).

doi: 10.1016/j.bmc.2003.09.025

[Abstract + Refs](#) [View at Publisher](#)

105. □ Zmazek, B., Žerovnik, J.

Computing the Weighted Wiener and Szeged Number on Weighted Cactus Graphs in Linear Time

(2003) *Croatica Chemica Acta*, 76 (2), pp. 137-143. [Cited 4 times](#).

[Abstract + Refs](#) [View at Publisher](#)

106. □ Thakur, A., Thakur, M., Khadikar, P.V., Supuran, C.T., Sudele, P.

QSAR study on benzenesulphonamide carbonic anhydrase inhibitors: Topological approach using Balaban index

(2004) *Bioorganic and Medicinal Chemistry*, 12 (4), pp. 789-793. [Cited 23 times](#).

doi: 10.1016/j.bmc.2003.10.058

[Abstract + Refs](#) [View at Publisher](#)

107. □ Thakur, M., Thakur, A., Khadikar, P.V.

QSAR studies on psychotomimetic phenylalkylamines

(2004) *Bioorganic and Medicinal Chemistry*, 12 (4), pp. 825-831. [Cited 4 times](#).

doi: 10.1016/j.bmc.2003.10.027

[Abstract + Refs](#) [View at Publisher](#)

108. □ Jaiswal, M., Khadikar, P.

QSAR Study on C NMR chemical shifts on carbinol carbon atoms

(2004) *Bioorganic and Medicinal Chemistry*, 12 (7), pp. 1793-1798. [Cited 7 times](#).

doi: 10.1016/j.bmc.2003.12.017

[Abstract + Refs](#) [View at Publisher](#)

109. □ Jaiswal, M., Khadikar, P.V., Supuran, C.T.

QSAR study on CA inhibitory activity of disulfonamides: Effect of halogen substitution

(2004) *Bioorganic and Medicinal Chemistry*, 12 (9), pp. 2477-2482. [Cited 12 times](#).

doi: 10.1016/j.bmc.2004.01.049

[Abstract + Refs](#) [View at Publisher](#)

110. □ Jaiswal, M., Khadikar, P.V., Scozzafava, A., Supuran, C.T.
(2004) *Bioorg. Med. Chem. Lett.*, 14, pp. 328-3290.

111. □ Khadikar, P.V., Singh, S., Jaiswal, M., Mandloi, D.

Topological estimation of electronic absorption bands of arene absorption spectra as a tool for modeling their toxicity and environmental pollution

(2004) *Bioorganic and Medicinal Chemistry Letters*, 14 (18), pp. 4795-4801. [Cited 4 times](#).

doi: 10.1016/j.bmcl.2004.06.094

[Abstract + Refs](#) [View at Publisher](#)

112. □ Jaiswal, M., Khadikar, P.V., Supuran, C.T.
Topological modeling of lipophilicity, diuretic activity, and carbonic inhibition activity of benzene sulfonamides: A molecular connectivity approach
(2004) *Bioorganic and Medicinal Chemistry Letters*, 14 (22), pp. 5661-5666. [Cited 8 times](#).
doi: 10.1016/j.bmcl.2004.08.051

[Abstract + Refs](#) [View at Publisher](#)

113. □ Joshi, S., Mandoli, D., Khadikar, P.V., Khosla, N.
(2004) *Bioinformatic India*, 2, pp. 92-99.
114. □ Thakur, M., Thakur, A., Khadikar, P.V., Supuran, C.T.
QSAR study on pK vis-à-vis physiological activity of sulfonamides: A dominating role of surface tension (inverse steric parameter)
(2005) *Bioorganic and Medicinal Chemistry Letters*, 15 (1), pp. 203-209. [Cited 11 times](#).
doi: 10.1016/j.bmcl.2004.10.032

[Abstract + Refs](#) [View at Publisher](#)

115. □ Muresan, S., Minailiuc, O., Diudea, M.V., Pejov, L.

Modeling herbicidal activity of phosphorus counting compounds by szeged indices

Rev. Roumaine Chim.

Personal communication

116. □ Khadikar, P.V., Sharma, V., Karmarkar, S., Supuran, C.T.
QSAR studies on benzene sulfonamide carbonic anhydrase inhibitors: Need of hydrophobic parameter for topological modeling of binding constants of sulfonamides to human CA-II

(2005) *Bioorganic and Medicinal Chemistry Letters*, 15 (4), pp. 923-930. [Cited 6 times](#).

doi: 10.1016/j.bmcl.2004.12.056

[Abstract + Refs](#) [View at Publisher](#)

117. □ Khadikar, P.V., Sharma, V., Karmarkar, S., Supuran, C.T.
Novel use of chemical shift in NMR as molecular descriptor: A first report on modeling carbonic anhydrase inhibitory activity and related parameters

(2005) *Bioorganic and Medicinal Chemistry Letters*, 15 (4), pp. 931-936. [Cited 9 times](#).

doi: 10.1016/j.bmcl.2004.12.057

[Abstract + Refs](#) [View at Publisher](#)

□

118. Khadikar, P.V., Sharma, V., Varma, R.G.
Novel estimation of lipophilicity using C NMR chemical shifts as molecular descriptor
(2005) *Bioorganic and Medicinal Chemistry Letters*, 15 (2), pp. 421-425. [Cited 5 times](#).
doi: 10.1016/j.bmcl.2004.10.075

[Abstract + Refs](#) [View at Publisher](#)

119. □ Mandoli, D., Joshi, S., Khadikar, P.V., Khosla, N.
(2005) *Bioorg. Med. Chem. Lett.*, 15, pp. 405-411. [Cited 2 times](#).

120. □ Jaiswal, M., Khadikar, P.V.
(2005) *J. Indian Chem. Soc.*, 82, pp. 1-3.

121. □ Agrawal, V.K., Gupta, M., Singh, J., Khadikar, P.V.
A novel method of estimation of lipophilicity using distance-based topological indices: Dominating role of equalized electronegativity
(2005) *Bioorganic and Medicinal Chemistry*, 13 (6), pp. 2109-2120. [Cited 2 times](#).
doi: 10.1016/j.bmc.2005.01.003

[Abstract + Refs](#) [View at Publisher](#)

122. □ Bonchev, D., Rouvray, D.H.

(2000) *Chemical Topology, Applications and Techniques*. [Cited 3 times](#).

Gordon and Breach: New York

123. □ Graovac, A., Gutman, I., Trinajstić, N.
(1977) *Topological Approach to the Chemistry of Conjugated Molecules*. [Cited 112 times](#).
Springer-Verlag, Berlin
124. □ Gutman, I., Polansky, O.
(1986) *Mathematical Concepts in Organic Chemistry*. [Cited 379 times](#).
Springer-Verlag, Berlin
125. □ Cvetković, D.M., Doob, M., Gutman, I., Torgasev, A.
(1988) *Recent Results in the Theory of Graph Spectra*
Elsevier. [Cited 42 times](#).
New York
126. □ Cyvin, S.J., Gutman, I.
(1988) *Kekulé Structures in Benzenoid Hydrocarbons*. [Cited 107 times](#).
Springer-Verlag, Berlin
127. □ Gutman, I., Cyvin, S.J.
(1989) *Introduction to the Theory of Benzenoid*

Hydrocarbons. [Cited 274 times](#).

Springer-Verlage, Berlin

128. □ Gutman, I.

Topological properties of benzenoid systems

(1992) *Topics in Current Chemistry*. [Cited 19 times](#).

Springer-Verlage, Berlin

129. □ Gutman, I.

Total pi-electron energy of benzenoid hydrocarbons

(1992) *Topics in Current Chemistry*

Springer-Verlage, Berlin

130. □ Ugi, I.

Computer chemistry

(1993) *Topics in Current Chemistry*

Springer-Verlage, Berlin

131. □ Gutman, I., Cyvin, S.J.

(1990) *Advances in the Theory of Benzenoid Hydrocarbons*. [Cited 19 times](#).

Springer-Verlage, Berlin

132. □ Gutman, I.

(1992) *Advances in the Theory of Benzenoid Hydrocarbons*

II. [Cited 19 times](#).

Springer-Verlage, Berlin

133. □ Diudea, M.V., Ivanciue, O.
(1995) *Molecular Topology*. [Cited 57 times](#).
Comlex, Cluj
134. □ Diudea, M.V., Khadikar, P.V.
Molecular Topology and Its Applications. [Cited 11 times](#).
Galgotia Pub. New Delhi, India (In press)
135. □ Diudea, M.V., Gutman, I., Jantschi, L.
(2001) *Molecular Topology*. [Cited 57 times](#).
Nova: Huntington
136. □ Gutman, I., Polansky, O.E.
(1986) *Mathematical Concepts in Organic Chemistry*. [Cited 379 times](#).
Springer-Verlag: Berlin
137. □ Trinajstić, N.
(1992) *Chemical Graph Theory, 2nd Revised Ed.* [Cited 7 times](#).
CRC Press, Boca Raton, FL
138. □ Trinajstić, N.
(1983) *Chemical Graph Theory, Vol. I & II*. [Cited 762 times](#).

CRC Press, Boca Raton, Fl

139. □ Chatterjee, S., Hadi, A.S., Price, B.
(2000) *Regression Analysis by Examples, 3rd Ed.* [Cited 679 times](#).
Wiley: New York
140. □ Green, J.R., Margerison, D.
Statistical treatment of experimental data
(1978) *Physical Sciences Data 2*
Elsevier, Amsterdam
141. □ Devillers, J., Karcher, W.
(1991) *Applied Multivariate Analysis in SAR and Environmental Studies, Vol. 2 in Chemical and Environmental Science, 2*.
Kluwer Academic, Dordrecht (The Netherlands)
142. □ Hansch, C.
(1978) *Correlation Analysis in Chemistry*. [Cited 73 times](#).
Chapman, N. B, Shorter, J. (Eds.) Plenum Press, NY
143. □ Draper, N., Smith, H.
(1966) *Applied Regression Analysis*. [Cited 5298 times](#).
J. Wiley and Sons: NY
144. □ Pogliani, L.

From molecular connectivity indices to semiempirical connectivity terms: Recent trends in graph theoretical descriptors

(2000) *Chemical Reviews*, 100 (10), pp. 3827-3858. [Cited 65 times](#).

doi: 10.1021/cr0004456

[Abstract + Refs](#) [View at Publisher](#)

145. □ Pogliani, L.

Modeling with special descriptors derived from a medium-sized set of connectivity indices

(1996) *Journal of Physical Chemistry*, 100 (46), pp. 18065-18077. [Cited 70 times](#).

[Abstract + Refs](#) [View at Publisher](#)

146. □ Todeschini, R.

Some Observations about the Pogliani Q Quality Factor

(2001) *Chemo Metrics Web News*

Milano Chemo metrics & QSAR Research Group

file:///C:/WINDOWS/Desktop/WebNews on Chemimotrics.

html. February

147. □ Pogliani, L.

Molecular connectivity descriptors of the

physicochemical properties of the α -amino acids

(1994) *Journal of Physical Chemistry*, 98 (5), pp. 1494-1499. [Cited 26 times](#).

[Abstract + Refs](#) [View at Publisher](#)

148. □ Todeschini, R., Consonni, V.
(2000) *Handbook of Molecular Descriptors*. [Cited 581 times](#).
Wiley-VCH, Weinheim (GER)
149. □ Karelson, M.
(2000) *Molecular Descriptors in QSAR/QSPR*. [Cited 175 times](#).
J. Wiley & Sons, New York
150. □ Diudea, M.V.
(2000) *QSPR/QSAR Studies by Molecular Descriptors*. [Cited 67 times](#).
Nova Science: Huntington
151. □ Basak, S.C., Gute, B.D., Grunwald, G.D.
(1998) *Quantitative Structure-Activity Relationships in Environmental Sciences VII*, 245
Eds. Chen, F., Schuurmann, SETAC Press, Pensacola, FL
152. □ Balaban, A.T.
QSAR and Computational Methods in Drug Discovery

(2000) *Encyclopedia of Analytical Chemistry*, 8, pp. 7288-7311. [Cited 6 times](#).

Meyers, R. A., Ed. Wiley, Chichester

153. □ Balaban, A.T.

(1997) *From Chemical Topology to Three-Dimensional Geometry*. [Cited 75 times](#).

Plenum Press: New York

154. □ Balaban, A.T.

(1976) *Chemical Applications of Graph Theory*. [Cited 202 times](#).

Academic Press, London (UK)

155. □ Devillers, J., Balaban, A.T.

(1999) *Topological Indices and Related Descriptors in QSAR and QSPR*. [Cited 233 times](#).

Gordon & Breach, Amsterdam (the Netherlands)

156. □ Das, A.

(1998) *Topological Modeling: Quantitative Structure - Activity Relationships*

Ph. D. Thesis, Devi Ahilya Vishwavidyalaya, Indore

157. □ Mandloi, M.

(1997) *Studies on Topological Modeling of Drug Activity*

Ph. D. Thesis, Devi Ahilya Vishwavidyalaya, Indore

158. □ Khadikar, Padmakar V., Pandharkar, Sadhana P.
X-RAY K-ABSORPTION EDGE ANALYSIS OF COBALT IN SOME COBALT COMPLEXES.

(1987) *Japanese Journal of Applied Physics, Part 1: Regular Papers & Short Notes*, 26 (7), pp. 1146-1152.

[Abstract + Refs](#) [View at Publisher](#)

159. □ Khadikar, P.V., Pandharkar, S.P.
Co-ordination Stoichimoetry, Edge-shift and Effective, Nuclear Charge: A Novel Correlation

(1986) *IL N Ouoto Cimento*, 8 D, pp. 33-38.

[View at Publisher](#)

160. □ Khadikar, P.V., Pandharkar, S.P.
(1986) *Thermochim. Acta*, 99, pp. 119-132.

[View at Publisher](#)

161. □ Khadikar, Padmaker V., Anikhindi, Ramesh G.
STRUCTURE AND CHEMICAL EFFECTS ON THE K-ABSORPTION EDGE OF COBALT IN SOME MIXED LIGAND COBALT COMPLEXES.

(1985) *Japanese Journal of Applied Physics, Part 1: Regular Papers & Short Notes*, 24 (11), pp. 1552-1554.

[Abstract + Refs](#) [View at Publisher](#)

162. □ Sharma, A.
(1999) *Structural Studies of Some Metal Chelates*. [Cited 2 times](#).
Ph. D. Thesis, Devi Ahilya Vishwavidyalaya, Indore
163. □ Saxena, A.
(2000) *Quantitative Structure - Activity Relationships for a Group of Sulfonamide Schiff's Base Inhibitors of Carbonic Anhydrase*
Ph. D. Thesis, Devi Ahilya Vishwavidyalaya, Indore
164. □ Buckley, F., Harary, F.
(1990) *Distance in Graphs*, Addison-Wesley: Redwood
165. □ Gutman, I.
(1973) *Studies on Topological Properties of Conjugated Hydrocarbons*
Ph. D. Thesis, University of Zagreb
166. □ Khaddar, T.
(2000) *Studies on Topology and Drug Activity*
Ph. D. Thesis, Devi Ahilya Vishwavidyalaya, Indore
167. □ Srivastava, R.C.
(2000) *Quantitative Structure - Activity Relationships on*

Some Anti-Hypertensive Drugs

Ph. D. Thesis, A. P. S. University, Rewa

168. □ Singh, N.
(2000) *QSAR Studies on Some Sulfa Drugs*
Ph. D. Thesis, A. P. S. University, Rewa
169. □ Sachan, S.
(2000) *Quantitative Structure - Activity Relationships on Some Antihistaminic Compounds*
Ph. D. Thesis, A. P. S. University, Rewa
170. □ Sikarwar, A.K.
(2001) *Studies on Spectra of Graphs of a Series of Salicylhydroxamic Acids*
Ph. D. Thesis, Devi Ahilya Vishwavidyalaya, Indore
171. □ Sharma, R.
(2002) *Studies on Some Sulfanilamide Schiff-Base Inhibitors*
Ph. D. Thesis, A. P. S. University, Rewa
172. □ Chaturvedi, S.
(2002) *QSAR Studies on Nonpolar Narcosis*
Ph. D. Thesis, A. P. S. University, Rewa
173. □ Sohgaura, R.
(2002) *On the Use of Topological Indices in QSAR Studies: A*

Case of Antitumor Drugs

Ph. D. Thesis, A. P. S. University, Rewa

174. □ Singh, J.

(2002) *On Topological Modeling of QSAR: A Multivariate Analysis*

Ph. D. Thesis, A. P. S. University, Rewa

175. □ Karmarkar, S.


(2002) *Topological Studies on Pesticides and Insecticides*

Ph. D. Thesis, A. P. S. University, Rewa

176. □ Jaiswal, M.

(2002) *Topological Modeling of Anti-inflammatory Agents*

Ph. D. Thesis, D. A. University, Indore

 Khadikar, P.V.; Research Division, Laxmi Fumigation and Pest Control, Pvt. Ltd., 3, Khatipura, Indore 452 007, India;
email: pvkhadikar@rediffmail.com

© Copyright 2006 Elsevier B.V., All rights reserved.

[Letters in Drug Design and Discovery](#)

Volume 2, Issue 8, December 2005, Pages 606-624

[Search History](#)

1 of 1

 [Live Chat](#)  [Help](#)  [Scopus Labs](#)

[About Scopus](#) | [Contact us](#) | [Terms & Conditions](#) | [Privacy Policy](#)

Copyright © 2007 [Elsevier B.V.](#) All rights reserved. Scopus® is a registered trademark of Elsevier B.V.