

Subhash C. Basak, Curriculum Vitae

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Present Position

Senior Research Associate
Center for Water and the Environment
Natural Resources Research Institute
5013 Miller Trunk Hwy
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Adjunct Professor
Department of Chemistry and
Department of Biochemistry & Molecular Biology
University of Minnesota Duluth
Duluth, MN 55812

Education

BS 1966 University of Calcutta, Chemistry
MS 1968 University of Calcutta, Biochemistry
PhD 1980 University of Calcutta, Biochemistry

Academic Appointments

July 2002 – present *Adjunct Professor*, Department of Biochemistry and Molecular Biology, University of Minnesota Duluth (UMD)
April 2001 – present *Adjunct Professor*, Department of Chemistry, UMD
July 1993 – present *Senior Research Associate*, Natural Resources Research Institute
Dec 1987 – Jun 1993 *Faculty Research Associate*, Natural Resources Research Institute, UMD
Jan 1982 – Nov 1987 *Faculty Research Associate*, Department of Chemistry, UMD
Jan 1970 – Dec 1981 *Assistant Professor*, Department of Chemistry, Charuchandra College, Calcutta, India

Teaching Experience

Department of Chemistry, Charuchandra College, Calcutta, India
Department of Biochemistry, University of Minnesota Duluth, 1988 – present
Toxicology PhD Program, University of Minnesota

Professional Affiliations

International Society for Mathematical Chemistry, President
International Academy for Mathematical Chemistry
International Association for Mathematical and Computer Modelling
International QSAR Society
American Chemical Society
New York Academy of Sciences
Society of Toxicology

Areas of Research Interest

Development of topological indices as molecular descriptors
Computer-assisted prediction of chemical genotoxicity
Structure-activity relationship (SAR) in drug design and environmental chemistry
Chemical graph theory and topology
Predictive toxicology
Mathematical chemistry

Honors and Awards

2004 ARA Journal Best Paper Award, American Romanian Academy of Arts and Sciences.
2004 Statistics in Chemistry Award, American Statistical Association.

Journal Editorial Board Memberships

SAR and QSAR in Environmental Research (Taylor & Francis)

Current Computer-Aided Drug Design (Bentham Science Publishers)

Open Medicinal Chemistry (Bentham Science Publishers)

Open Proteomics Journal (Bentham Science Publishers)

ARKIVOC (Bentham Science Publishers)

Past board member, *Journal of Chemical Information and Modeling* (American Chemical Society)

Consultancy

Consultant to the Upjohn Company, Kalamazoo, Michigan, 1986–1988.

Consultant, Research and Evaluation Associated, North Carolina.

Consultant, BioPred, Montana, 2005–2007.

Chairperson for International Conferences

1. *Co-Chairperson* of the Third Indo-US Lecture Series on Discrete Mathematical Chemistry, Tiruchirappalli, Tamil Nadu, India, January 7–10, 2008.
2. *Co-Chairperson* of the Second Indo-US Lecture Series on Discrete Mathematical Chemistry, Kalpetta, Kerala, India, June 20–25, 2007.
3. *Chaired* a session at the International Academy of Mathematical Chemistry (IAMC) 2007 conference held in Dubrovnik, Croatia, June 7–10, 2007.
4. *Co-Chairperson* of the First Indo-US Lecture Series on Discrete Mathematical Chemistry, Bangalore, Karnataka, India, January 8–11, 2007.
5. *Chaired* the session “Modeling of Bioactive Molecules” at the 21st Dubrovnik International Course and Conference on the Interfaces Among Mathematics, Chemistry and Computer Sciences (Math/Chem/Comp 2006), Dubrovnik, Croatia, June 19–24, 2006.
6. *Chaired* a session on Environmental Fate Modeling at the 12th International Workshop on Quantitative Structure-Activity Relationships in Environmental Chemistry (QSAR 2006) in Lyon, France, May 8–12.
7. *Co-Chairperson* of a QSAR and Predictive Molecular Modeling session at the Computational Methods in Toxicology and Pharmacology conference held in Shanghai, October 29–November 1, 2005.
8. *Chaired* a session on Mathematical Chemistry and QSAR at the International Conference of Computational Methods in Sciences and Engineering 2005" in Korinthos, Greece, October 21–26, 2005.
9. *Chaired* a session at Conferentia Chemometrica 2005 in Hajdúszoboszló, Hungary, August 28–30.
10. *Co-Chairperson* of the Fourth Indo-US Workshop on Mathematical Chemistry, Pune, Maharashtra, India, January 8–12, 2005.
11. *Chaired* a session at the Sixth Girona Seminar on Molecular Similarity, July 21–24, 2004, organized at the University of Girona, Spain.
12. *Chaired* a session at the Chemoinformatics Symposium at the Intelligent Drug Discovery and Development Conference, May 28-30, 2004, organized by the Cambridge Health Institute, Philadelphia, Penn.
13. *Co-Chairperson* of the session “Toxicogenomics and Molecular Mechanisms” at the 11th International Workshop on Quantitative Structure-Activity Relationships in the Human Health and Environmental Sciences, Liverpool, England, May 2004.
14. *Chaired* a session at the International Symposium on Water: Crisis and Strategies, organized jointly by the International Institute of Bengal Basin and Center for Ground Water Studies in Kolkata, India, February 7–8, 2004.
15. *Co-Chairperson* of the Third Indo-US Workshop on Mathematical Chemistry, Duluth, Minnesota, August 2–7, 2003.
16. *Co-Chairperson* of the Second Indo-US Workshop on Mathematical Chemistry, Duluth, Minnesota, May 30–June 3, 2000.
17. *Co-Chairperson* of the First Indo-US Workshop on Mathematical Chemistry, West Bengal India, January 9–13, 1998.
18. *Chaired* the session “Mathematical Modelling in Drug Design and Risk Assessment” at the Tenth International Conference Mathematical and Computer Modelling and Scientific Computing held in Boston,

July 5–8, 1995.

19. *Chaired* the session “Computational Approaches to Molecular Design” at the Ninth International Conference on Mathematical and Computer Modelling, University of California, Berkeley, CA, July 26–29, 1993.
20. *Chaired* a session entitled “Multivariate and Molecular Similarity Analysis” at QSAR ‘92, Duluth Minnesota, 1992.
21. *Organized and chaired* a session entitled “Mathematical Modelling in Molecular Design and Hazard Assessment” at the Eighth International Conference on Mathematical and Computer Modelling held in Maryland, April 1–4, 1992.
22. *Organized and chaired* a session entitled “Mathematical Modelling Molecular Design” at the Seventh International Conference on Mathematical and Computer Modelling held in Chicago, August 2–5, 1989.
23. *Organized and chaired* two sessions entitled “Mathematical Modelling in Drug Design” at the Sixth International Conference on Mathematical Modelling, held at the Washington University, St. Louis, during August 3–7, 1987.

Grants and Contracts (Total received — \$7,466,017)

1. Development of QSAR methods to predict the biological interaction of non-traditional nerve agents (NTAs) via blood-tissue partitioning, Defense Threat Reduction Agency/Henry Jackson Foundation, \$681,000, 6/07 – 6/09 (Principal Investigator).
2. Predicting chemical toxicity from proteomics and computational chemistry: An integrated approach, US Air Force Office of Scientific Research, \$623,579, 7/05 – 1/08 (Principal Investigator).
3. Behavior-modifying compounds for disease vector control, US Department of Agriculture, \$1,391,485, 6/04 – 9/08 (Principal Investigator).
4. Predicting toxicity of chemical mixtures using structural, genomics and proteomics based descriptors: An integrated approach, Agency for Toxic Substances and Disease Registry, \$180,998, 9/02 – 9/07 (Principal Investigator).
5. Use of biodescriptors and chemodescriptors in predictive toxicology: A mathematical/ computational approach, US Air Force Office of Scientific Research, \$899,679, 3/02 – 2/05 (Principal Investigator).
6. Integration of biodescriptors and chemodescriptors for predictive toxicology: A mathematical/ computational approach, US Air Force Office of Scientific Research, \$179,999, 11/00 – 10/01 (Principal Investigator).
7. Design of novel and environmentally benign photoactive chemicals, Minnesota Technology, Inc., \$53,686, 7/99 – 6/02 (Principal Investigator).
8. Computer-assisted design of environmentally benign photoactive chemicals, Minnesota Technology, Inc., \$59,953, 7/97 – 6/99 (Principal Investigator).
9. Prediction of health and environmental hazard of chemicals: A hierarchical approach using QMSA and QSAR, US Air Force Office of Scientific Research, \$518,514, 7/97 – 6/00 (Principal Investigator).
10. Prediction of environmental toxicity of chemicals using molecular similarity and hierarchical QSAR, Exxon Corp. \$150,062, 1/90 – 12/96 (Principal Investigator).
11. AASERT 96 - Quantitative characterization of molecular similarity spaces: Tools for computational toxicology, US Air Force Office of Scientific Research, \$167,540, 7/96 – 6/99 (Principal Investigator).
12. Prediction of environmental toxicity of chemicals using molecular similarity, Ciba-Geigy Corporation, \$30,000, 9/91 – 8/95 (Principal Investigator).
13. Predicting toxicity and degradability of quadricyclane, fluorocarbon ethers and their analogs, US Air Force Office of Scientific Research, \$641,131, 7/94 – 6/97 (Principal Investigator).
14. Computational techniques to quantify chemical similarity: tools for risk assessment, US Environmental Protection Agency, \$333,723, 7/92 – 6/95 (Principal Investigator).
15. Structure-activity relationships (SAR) for anti-convulsant drug development, National Institute of Neurological Disorders and Stroke, NIH, \$1,171,060, 10/90 – 6/94 (Principal Investigator).
16. Assessment of environmental toxicity of chemicals from structure: A computational approach, US Environmental Protection Agency, \$130,000, 5/89 – 5/91 (Principal Investigator).
17. Software development-prediction model for carcinogenicity and mutagenicity of organic chemicals, Greater Minnesota Corporation, \$90,000, 12/88 – 6/91 (Principal Investigator).
18. Development of knowledge-based expert system for evaluating chemical carcinogens, US Environmental

Publications (Total — 201)

A. Brain biochemistry, pesticide biochemistry and analytical biochemistry (8 total)

1. Effects of acute and multiple dose administration of sumithion on some enzymes of *Periplanata Americana* (Linn), R. Sengupta, S.C. Basak, D. Sarkar, and J.J. Ghosh, *Pest. Biochem. Physiol.*, 5, 52–53 (1975).
2. A simplified colorimetric method for determination of arylamidase activity, D. Sarkar, S.C. Basak, and J.J. Ghosh, *Indian J. Biochem. Biophys.*, 13, 245–247 (1976).
3. Comparative studies of the brain and blood enzymes in rats after single and multiple dose of morphine administration, B. Banerjee, S.C. Basak, and J.J. Ghosh, *Brain News*, 12, 18–21 (1980).
4. Plasma target enzyme desensitization following chronic morphine treatment in rats, B. Banerjee, S.C. Basak, and J.J. Ghosh, *IRCS Med. Sci.*, 9, 929–630 (1981).
5. Amphetamine-induced alterations in the target enzymes: Possibility of a dual role in adaptation, S.C. Basak and J.J. Ghosh, *IRCS Med. Sci.*, 10, 419–420 (1982).
6. Chronic amphetamine toxicity: Search for biochemical correlates at the level of cerebral target enzymes, S.C. Basak and J.J. Ghosh, *IRCS Med. Sci.*, 10, 675–676 (1982).
7. Pethidine-induced desensitization of plasma target enzyme in rate, B. Banerjee, S.C. Basak, and J.J. Ghosh, *IRCS Med. Sci.*, 10, 73–74 (1982).
8. The significance of blood cholinesterase systems in monitoring morphine tolerance, B. Banerjee, S.C. Basak, and J.J. Ghosh, *Indian J. Med. Res.*, 75, 422–472 (1982).

B. Development of topological descriptors for structure-activity relationships (SAR) (2 total)

9. Study of the structure-function relationship of pharmacological and toxicological agents using information theory, S.C. Basak, A.B. Roy, and J.J. Ghosh, in *Proceedings of the Second International Conference on Mathematical Modelling*, X.J.R. Avula, R. Bellman Y.L. Luke and A.K. Rigler, Eds., pp 851–856, University of Missouri-Rolla, Rolla, Missouri (1979).
10. Molecular topology and narcosis: A quantitative structure-activity relationship (QSAR) study of alcohols using complementary information content (CIC), S.C. Basak and V.R. Magnuson, *Arzneim.-Forsch./Drug Res.*, 33, 501–503 (1983).

C. Quantitative structure-activity relationship (QSAR) studies using physicochemical and topological descriptors (147 total)

11. Quantitative structure-activity relationships (QSAR) studies of pharmacological agents using topological information content. C. Raychaudhury, S.C. Basak, A.B. Roy, and J.J. Ghosh, *Indian Drugs*, 18, 97–102 (1980).
12. A quantitative structure-activity relationship (QSAR) study of barbiturates, spasmolytic, and diphenhydramines using van der Waals' volume, S.K. Ray, S.C. Basak, C. Raychaudhury, A.B. Roy, and J.J. Ghosh, *Acta Ciencia Indica*, vol VII c., 4, 187–192 (1981).
13. Quantitative structure-activity relationship studies of bioactive molecules using structural information indices, S.K. Ray, S.C. Basak, C. Raychaudhury, A.B. Roy, and J.J. Ghosh, *Indian J. Chem.*, 20B, 894–897 (1981).
14. Molecular connectivity and antifungal activity: A QSAR study of substituted phenols against skin pathogens, A.K. Samanta, S.K. Ray, S.C. Basak, and A.D. Bose, *Arzneim.-Forsch./Drug Res.*, 32, 1515–1517 (1982).
15. Molecular topology and pharmacological action: A QSAR study of tetrazoles using structural information content, S.C. Basak, S.K. Ray, C. Raychaudhury, A.B. Roy, and J.J. Ghosh, *IRCS Med. Sci.*, 10, 145–146 (1982).
16. A quantitative structure-activity relationship (QSAR) analysis of carbamoyl piperidines, barbiturates and alkanes using information-theoretic topological indices, S.K. Ray, S.C. Basak, C. Raychaudhury, A.B. Roy, and J.J. Ghosh, *Ind. J. Pharmac.*, 13, 301–312, (1982).

17. A quantitative structure-activity relationship study of N-alkylnerketobemidones and triazonones using structural information content, S.K. Ray, S.C. Basak, C. Raychaudhury, A.B. Roy, and J.J. Ghosh, *Arzneim.-Forsch./Drug Res.*, 32, 322–325 (1982).
18. A quantitative structure-activity relationship study of tumor inhibitory triazenes using bonding information content and lipophilicity, S.K. Ray, S.C. Basak, C. Raychaudhury, A.B. Roy, and J.J. Ghosh, *IRCS Med. Sci.*, 10, 933–934 (1982).
19. Structure-activity relationships and pharmacokinetics : A comparative study of hydrophobicity, van der Waals' volume and topological parameters, S.C. Basak, D.P. Gieschen, V.R. Magnuson, and D.K. Harriss, *IRCS Med. Sci.*, 10, 619–620 (1982).
20. Physicochemical and topological correlates of enzymatic acetyl transfer reaction, S.C. Basak, D.P. Gieschen, D.K. Harriss, and V.R. Magnuson, *J. Pharm. Sci.*, 72, 934–937 (1983).
21. The utility of information content, structural information content, hydrophobicity and van der Waals' volume in the design of barbiturates and tumor-inhibitory triazenes: A comparative study, S.K. Ray, S.C. Basak, C. Raychaudhury, A.B. Roy, and J.J. Ghosh, *Arzneim.-Forsch./Drug Res.*, 33, 352–356 (1983).
22. Comparative study of lipophilicity versus topological molecular descriptors in biological correlations, S.C. Basak, D.K. Harriss, and V.R. Magnuson, *J. Pharm. Sci.*, 73, 429–437 (1984).
23. Discrimination of isomeric structures using information-theoretic topological indices, C. Raychaudhury, S.K. Ray, J.J. Ghosh, A.B. Roy, and S.C. Basak, *J. Comput. Chem.*, 5, 581–588 (1984).
24. A quantitative correlations of the LC50 values of esters in *Pimephales promelas* using physicochemical and topological parameters, S.C. Basak, D.P. Gieschen, and V.R. Magnuson, *Environ Toxicol. Chem.*, 3, 191–199 (1984).
25. Weighted information indices & anxioselective anxiolytic drug design, S.K. Ray, S. Gupta, S.C. Basak, C. Raychaudhury, A.B. Roy, and J.J. Ghosh, *Indian J. Chem.*, 24B, 1149–1153 (1985).
26. A comparative study of lipophilicity and topological indices in biological correlation, S.C. Basak, L.J. Monsrud, M.E. Rosen, C.M. Frane, and V.R. Magnuson, *Acta Pharm. Yugosl.: special volume on QSAR in drug research*, A. Sabljic, D. Plavsic, and N. Trinajstic (Eds.), 36, 81–95 (1986).
27. Molecular topology and mutagenicity: A QSAR study of nitrosamines, S.C. Basak, C.M. Frane, M.E. Rosen, and V.R. Magnuson, *IRCS Med. Sci.*, 14, 848–849 (1986).
28. Molecular topology and acute toxicity: A QSAR study of monoketones, S.C. Basak, C.M. Frane, M.E. Rosen, and V.R. Magnuson, *Med. Sci. Res.*, 15, 887–888 (1987).
29. Topological indices: their nature, mutual relatedness, and applications, S.C. Basak, V.R. Magnuson, G.J. Niemi, R.R. Regal, and G.D. Veith, *Mathematical Modelling*, 8, 300–305 (1987).
30. Binding of barbiturates to cytochrome P450: a QSAR study using log P and topological indices, S.C. Basak, *Med. Sci. Res.*, 16, 281–282 (1988).
31. A characterization of molecular similarity methods for property prediction, M. Johnson, S.C. Basak, and G. Maggiora, *Mathl. Comput. Modelling*, 11, 630–634 (1988).
32. Determining structural similarity of chemicals using graph-theoretic indices, S.C. Basak, V.R. Magnuson, G.J. Niemi, and R.R. Regal, *Discrete Appl. Math.*, 19, 17–44, (1988); Special volume: Applications of Graph Theory in Chemistry and Physics, J.W. Kennedy and L.V. Quintas (Eds.).
33. A graph-theoretic approach to predicting molecular properties, S.C. Basak, G.J. Niemi, and G.D. Veith, *Mathl. Comput. Modelling*, 14, 511–516 (1990).
34. Optimal characterization of structure for prediction of properties, S.C. Basak, G.J. Niemi, and G.D. Veith, *J. Math. Chem.*, 4, 185–205 (1990).
35. Predicting properties of molecules using graph invariants, S.C. Basak, G.J. Niemi, and G.D. Veith, *J. Math. Chem.*, 7, 243–272 (1991).
36. Prediction of octanol-water partition coefficient (K_{OW}) using algorithmically-derived variables, G.J. Niemi, S.C. Basak, G.D. Veith, and G. Grunwald, *Environ. Toxicol. Chem.*, 11, 891–898 (1992).
37. A comparative study of graph invariants, total surface area, and volume in predicting boiling points of alkanes, S.C. Basak and G.D. Grunwald, *Mathl. Modelling Sci. Computing*, 2, 735–740 (1993).
38. Application of graph theoretical parameters in quantifying molecular similarity and structure-activity

- studies, S.C. Basak, S. Bertelsen, and G. Grunwald, *J. Chem. Inf. Comput. Sci.*, 34, 270–276 (1994).
39. Correlation between structure and normal boiling points of haloalkanes C₁-C₄ using neural networks, A.T. Balaban, S.C. Basak, T. Colburn, and G.D. Grunwald, *J. Chem. Inf. Comput. Sci.*, 34, 1118–1121 (1994).
 40. Molecular similarity and risk assessment: analog selection and property estimation using graph invariants, S.C. Basak and G.D. Grunwald, *SAR QSAR Environ. Res.*, 2, 289–307 (1994).
 41. New centric topological indexes for acyclic molecules (trees) and substituents (rooted trees) and coding of rooted trees, A.T. Balaban, S. Bertelsen, and S.C. Basak, *Math. Chem. (MATCH)*, 30, 55–72 (1994).
 42. Use of topological space and property space in selecting structural analogs, S.C. Basak and G.D. Grunwald, *Mathl. Modelling Sci. Computing*, 4, 464–469 (1994).
 43. Estimation of lipophilicity from molecular structural similarity, S.C. Basak and G.D. Grunwald, *New J. Chem.*, 19, 231–237 (1995).
 44. Molecular similarity and estimation of molecular properties, S.C. Basak and G.D. Grunwald, *J. Chem. Inf. Comput. Sci.*, 35, 366–372 (1995).
 45. Predicting mutagenicity of chemicals using topological and quantum chemical parameters: A similarity based study, S.C. Basak and G.D. Grunwald, *Chemosphere*, 31, 2529–2546 (1995).
 46. Tolerance space and molecular similarity, S.C. Basak and G.D. Grunwald, *SAR QSAR Environ. Res.*, 3, 265–277 (1995).
 47. Use of graph theoretic parameters in risk assessment of chemicals, S.C. Basak, S. Bertelsen, and G.D. Grunwald, *Toxicol. Lett.*, 79, 239–250 (1995).
 48. A comparative study of topological and geometrical parameters in estimating normal boiling point and octanol-water partition coefficient, S.C. Basak, B.D. Gute, and G.D. Grunwald, *J. Chem. Inf. Comput. Sci.*, 36, 1054–1060 (1996).
 49. Estimation of normal boiling points of haloalkanes using molecular similarity, S.C. Basak, B.D. Gute and G.D. Grunwald, *Croat. Chim. Acta*, 69, 1159–1173 (1996).
 50. Predicting blood-brain transport of drugs: A computational approach. S.C. Basak, B.D. Gute, and L.R. Drewes, *Pharm. Res.*, 13, 775–778 (1996).
 51. A new QSAR algorithm combining principal component analysis with a neural network: Application to calcium channel antagonists. Viswanadhan, V. N.; Muellera, G. A.; Basak, S. C.; Weinstein, J. N. <http://www.netsci.org/Science/Compchem/feature07.html> (1996).
 52. Characterization of molecular structures using topological indices, S.C. Basak and B.D. Gute, *SAR QSAR Environ. Res.*, 7, 1–21 (1997).
 53. Computational study of the environmental fate of selected aircraft fuel system deicing compounds, G.W. Mushrush, S.C. Basak, J.E. Slone, E.J. Beal, S. Basu, W.M. Stalick, and D.R. Hardy, *J. Environ. Sci. Health*, A32, 2201–2211 (1997).
 54. Predicting acute toxicity of benzene derivatives using theoretical molecular descriptors: a hierarchical QSAR approach, B.D. Gute and S.C. Basak, *SAR QSAR Environ. Res.*, 7, 117–131 (1997).
 55. Use of topostructural, topochemical, and geometric parameters in the prediction of vapor pressure: A hierarchical approach, S.C. Basak, B.D. Gute, and G.D. Grunwald, *J. Chem. Inf. Comput. Sci.*, 37, 651–655 (1997).
 56. Characterization of isospectral graphs using graph invariants and derived orthogonal parameters, K. Balasubramanian and S.C. Basak, *J. Chem. Inf. Comput. Sci.*, 38, 367–373 (1998).
 57. A comparative study of molecular similarity, statistical and neural network methods for predicting toxic modes of action of chemicals, S.C. Basak, G.D. Grunwald, G.E. Host, G.J. Niemi, and S.P. Bradbury, *Environ. Toxicol. Chem.*, 17, 1056–1064 (1998).
 58. Assessment of the mutagenicity of aromatic amines from theoretical structural parameters: A hierarchical approach, S.C. Basak, B.D. Gute and G.D. Grunwald, *SAR QSAR Environ. Res.*, 10, 117–129 (1999).
 59. Correlation between structure and normal boiling points of acyclic carbonyl compounds, A.T. Balaban, D. Mills and S.C. Basak, *J. Chem. Inf. Comput. Sci.*, 39, 758–764 (1999).

60. Hazard assessment modeling: An evolutionary ensemble approach, D. Opitz, S. Basak and B.D. Gute, *Genetic and Evolutionary Computation*, 2, 1643–1651 (1999).
61. Prediction of complement inhibitory activity of benzamidines using topological and geometrical parameters, S.C. Basak, B.D. Gute, and S. Ghatak, *J. Chem. Inf. Comput. Sci.*, 39, 255–260 (1999).
62. Normal boiling points of 1, ω -Alkanedinitriles: The highest increment in a homologous series, A.T. Balaban, S.C. Basak, and Denise Mills, *J. Chem. Inf. Comput. Sci.*, 39, 769–774 (1999).
63. Optimal molecular descriptors based on weighted path numbers, M. Randić and S.C. Basak, *J. Chem. Inf. Comput. Sci.*, 39, 261–266 (1999).
64. Prediction of the dermal penetration of polycyclic aromatic hydrocarbons (PAHs): A hierarchical QSAR approach, B.D. Gute, G.D. Grunwald, and S.C. Basak, *SAR QSAR Environ. Res.*, 10, 1–15 (1999).
65. A comparative QSAR study of benzamidines complement-inhibitory activity and benzene derivatives acute toxicity, S.C. Basak, B.D. Gute, B. Lucic, S. Nikolic and N. Trinajstić, *Computers and Chemistry*, 24, 181–191 (2000).
66. Construction of high-quality structure-property-activity regressions: The boiling points of sulfides, M. Randić and S.C. Basak, *J. Chem. Inf. Comput. Sci.*, 40, 899–905 (2000).
67. Multiple regression analysis with optimal descriptors, M. Randić and S.C. Basak, *SAR QSAR Environ. Res.*, 11, 1–23 (2000).
68. On 3-D graphical representation of DNA primary sequences and their numerical characterization, M. Randić, M. Vracko, A. Nandy, and S.C. Basak, *J. Chem. Inf. Comput. Sci.*, 40, 1235–1244 (2000).
69. On characterization of physical properties of amino acids, M. Randić, D. Mills and S.C. Basak, *Int. J. Quant. Chem.*, 80, 1199–1209 (2000).
70. On ordering of folded structures, M. Randić, M. Vracko, M. Novic and S.C. Basak, *Mathematical Chemistry, MATCH*, 42, 181–231 (2000).
71. QSPR modeling: Graph connectivity indices versus line graph connectivity indices, S.C. Basak, S. Nikolic, N. Trinajstić, D. Amic and D. Beslo, *J. Chem. Inf. Comput. Sci.*, 40, 927–933 (2000).
72. Reverse Wiener indices, A.T. Balaban, D. Mills, O. Ivanciuc, and S.C. Basak, *Croat. Chim. Acta*, 73, 923–941 (2000).
73. A simple numerical descriptor for quantifying effect of toxic substances on DNA sequences, A. Nandy and S.C. Basak, *J. Chem. Inf. Comput. Sci.*, 40, 915–919 (2000).
74. Topological indices: Their nature and mutual relatedness, S.C. Basak, A.T. Balaban, G.D. Grunwald and B.D. Gute, *J. Chem. Inf. Comput. Sci.*, 40, 891–898 (2000).
75. Use of statistical and neural net approaches in predicting toxicity of chemicals, S.C. Basak, G.D. Grunwald, B.D. Gute, K. Balasubramanian and D. Opitz, *J. Chem. Inf. Comput. Sci.*, 40, 885–890 (2000).
76. Characterization of DNA primary sequences based on the average distance between bases, M. Randić and S.C. Basak, *J. Chem. Inf. Comput. Sci.*, 41, 561–568 (2001).
77. Comparison of a neural net-based QSAR algorithm (PCANN) with hologram- and multiple linear regression-based QSAR approaches: Application to 1,4-dihydropyridine-based calcium channel antagonists, V.N. Viswanadhan, G.A. Muellera, S.C. Basak and J.N. Weinstein, *J. Chem. Inf. Comput. Sci.*, 41, 505–511 (2001).
78. Distance indices and their hyper-counterparts: Intercorrelation and use in the structure-property modeling, N. Trinajstić, S. Nikolic, S.C. Basak and I. Lukovits, *SAR QSAR Environ. Res.*, 12, 31–54 (2001).
79. Interpretation of quantitative structure-property and -activity relationships, A.R. Katritzky, R. Putrukhin, D. Tatham, S. Basak, E. Benfenati, M. Karelson, and U. Maran, *J. Chem. Inf. Comput. Sci.*, 41, 679–685 (2001).
80. Molecular similarity based estimation of properties: A comparison of structure spaces and property spaces, B.D. Gute, G.D. Grunwald, D. Mills and S.C. Basak, *SAR QSAR Environ. Res.*, 11, 363–382 (2001).

81. Molecular similarity-based estimation of properties: A comparison of three structure spaces, B.D. Gute and S.C. Basak, *J. Mol. Graphics and Modelling*, 20, 95–109 (2001).
82. A new descriptor for structure-property and structure-activity correlations, M. Randic and S.C. Basak, *J. Chem. Inf. Comput. Sci.*, 41, 650–656 (2001).
83. A novel 2-D graphical representation of DNA sequences of low degeneracy, X. Guo, M. Randic and S.C. Basak, *Chem. Phys. Lett.*, 350, 106–112 (2001).
84. On characterization of proteomics maps and chemically induced changes in proteomes using matrix invariants: Application to peroxisome proliferators, M. Randic, F. Witzmann, M. Vracko and S.C. Basak, *Med. Chem. Res.*, 10, 456–479 (2001).
85. On structural interpretation of several distance related topological indices, M. Randic, A.T. Balaban, and S.C. Basak, *J. Chem. Inf. Comput. Sci.*, 41, 593–601 (2001).
86. On the characterization of DNA primary sequences by triplet of nucleic acid bases, M. Randic, X. Guo, and S.C. Basak, *J. Chem. Inf. Comput. Sci.*, 41, 619–626 (2001).
87. On use of the variable connectivity index $1\chi_f$ in QSAR: Toxicity of aliphatic ethers, M. Randic and S.C. Basak, *J. Chem. Inf. Comput. Sci.*, 41, 614–618 (2001).
88. Prediction of gas chromatographic retention indices using variable connectivity index, M. Randic, S.C. Basak, M. Pompe and M. Novic, *Acta Chim. Slov.*, 48, 169–180 (2001).
89. Prediction of mutagenicity of aromatic and heteroaromatic amines from structure: A hierarchical QSAR approach, S.C. Basak, D.R. Mills, A.T. Balaban, and B.D. Gute, *J. Chem. Inf. Comput. Sci.*, 41, 671–678 (2001).
90. Prediction of mutagenicity utilizing a hierarchical QSAR approach, S.C. Basak and D. Mills, *SAR QSAR Environ. Res.*, 12, 481–496 (2001).
91. Quantitative structure-property relationships (QSPRs) for the estimation of vapor pressure: A hierarchical approach using mathematical structural descriptors, S.C. Basak and D. Mills, *J. Chem. Inf. Comput. Sci.*, 41, 692–701 (2001).
92. QSAR with few compounds and many features, D. Hawkins, S. Basak, and X. Shi, *J. Chem. Inf. Comput. Sci.*, 41, 663–670 (2001).
93. Use of mathematical structural invariants in the development of QSPR models, S.C. Basak and D. Mills, *MATCH (Commun. Math. Comput. Chem.)*, 44, 15–30 (2001).
94. Alkane ordering as a criterion for similarity between topological indices: Index J as a "sharpened Wiener index," A.T. Balaban, D. Mills and S.C. Basak, *MATCH (Commun. Math. Comput. Chem.)*, 45, 5–26 (2002).
95. A comparative study of proteomics maps using graph theoretical biodescriptors, M. Randic and S. C. Basak, *J. Chem. Inf. Comput. Sci.*, 42, 983–992 (2002).
96. Novel matrix invariants for characterization of changes of proteomics maps, M. Randic, J. Zupan, M. Novic, B.D. Gute, and S.C. Basak, *SAR QSAR Environ. Res.*, 13, 689–703 (2002).
97. Prediction of tissue:air partition coefficients: A comparison of structure-based and property-based methods, S.C. Basak, D. Mills, D.M. Hawkins, H.A. El-Masri, *SAR QSAR Environ. Res.*, 13, 649–665 (2002).
98. QSAR modeling of flotation collectors using principal components extracted from topological indices, R. Natarajan, I. Nirdosh, S. C. Basak and D. R. Mills, *J. Chem. Inf. Comput. Sci.*, 42, 1425–1430 (2002).
99. Quantitative descriptor for SNP related gene sequences, A. Nandy, P. Nandy, and S.C. Basak, *Internet Electron. J. Mol. Des.*, 1, 367–373 (2002), <http://www.biochempress.com>.
100. Quantitative molecular similarity analysis (QMSA) methods for property estimation: A comparison of property-based, arbitrary, and tailored similarity spaces, S.C. Basak, B.D. Gute, D. Mills, *SAR QSAR Environ. Res.*, 13, 727–742 (2002).
101. Structure-water solubility modeling of aliphatic alcohols using the weighted path numbers, D. Amic, S.C. Basak, B. Lucic, S. Nikolic and N. Trinajstic, *SAR QSAR Environ. Res.*, 13, 281–295 (2002).
102. Tailored similarity spaces for the prediction of physicochemical properties, B.D. Gute, S.C. Basak, D.

- Mills, and D.M. Hawkins, *Internet Electronic J. Mol. Design*, 1, 374–387 (2002), <http://www.biochempress.com/>.
103. Assessing model fit by cross-validation, D. M. Hawkins, S. C. Basak, D. Mills, *J. Chem. Inf. Comput. Sci.*, 43, 579–586 (2003).
 104. How and why did our view of the world change during the last six hundred years? A. T. Balaban, S. C. Basak, *Amer. Romanian Acad. J.*, 28, 25–35 (2003).
 105. Novel map descriptors for characterization of toxic effects in proteomics maps, Z. Bajzer, M. Randić, D. Plavšić, S.C. Basak, *J. Molecular Graphics and Modelling*, 22, 1–9 (2003).
 106. Prediction of cellular toxicity of halocarbons from computed chemodescriptors: A hierarchical QSAR approach, S.C. Basak, K. Balasubramanian, B.D. Gute, D. Mills, A. Gorczynska, and S. Roszak. *J. Chem. Inf. Comput. Sci.*, 43, 1103–1109 (2003).
 107. Prediction of human blood:air partition coefficient: A comparison of structure-based and property-based methods, Subhash C. Basak, Denise Mills, Douglas M. Hawkins, and Hisham A. El-Masri, *Risk Analysis*, 23, 1173–1184 (2003).
 108. Quantitative molecular similarity methods in the property/ toxicity estimation of chemicals: A comparison of arbitrary versus tailored similarity spaces, S. C. Basak, B. D. Gute, D. Mills and D. M. Hawkins, *J. Mol. Struct. THEOCHEM*, 622, 127–145 (2003).
 109. Use of topological indices in predicting aryl hydrocarbon (Ah) receptor binding potency of dibenzofurans: A hierarchical QSAR approach. S.C. Basak, D. Mills, M. M. Mumtaz and K. Balasubramanian. *Indian. J. Chem.*, 42A, 1385–1391 (2003).
 110. Characterization of 2-D proteome maps based on the nearest neighborhoods of spots, M. Randić, Lers, N., D. Plavšić, S. C. Basak, *Croat. Chem. Acta*, 77, 345–351 (2004).
 111. Chemodescriptors versus biodescriptors for toxicity prediction on halocarbons, B.D. Gute, S.C. Basak, K. Balasubramanian, K. Geiss, and D.M. Hawkins, *Environ. Toxicol. Pharmacol.*, 16, 121–129 (2004).
 112. Counter-propagation artificial neural network as a tool for the independent variable selection: Structure-mutagenicity study on aromatic amines, A. Jezierska, M. Vracko, S. C. Basak, *Mol. Diversity*, 8, 371–377 (2004).
 113. Interrelationship of major topological indices evidenced by clustering, S. C. Basak, B. D. Gute, and A. T. Balaban, *Croat. Chem. Acta*, 77, 331–344 (2004).
 114. Modeling of structure-mutagenicity relationship: counter propagation neural network approach using calculated structural descriptors, I.V. Valkova, M. Vracko, S.C. Basak, *Anal. Chim. Acta*, 509, 179–186 (2004).
 115. On invariants of a 2-D proteome map derived from neighborhood graphs. Randić, M.; Lers, N.; Plavšić, D.; Basak, S. C. *J. Proteom. Res.*, 3, 778–785 (2004).
 116. On similarity of proteome maps, M. Randić and S. C. Basak, *Med. Chem. Res.*, 13, 800–811 (2004).
 117. Predicting blood:air partition coefficients using theoretical molecular descriptors, S. C. Basak, D. Mills, H. A. El-Masri, M. M. Mumtaz, and D. M. Hawkins, *Environ. Toxicol. Pharmacol.*, 16, 45–55 (2004).
 118. QSARs for chemical mutagens from structure: ridge regression fitting and diagnostics, D. M. Hawkins, S. C. Basak, and D. Mills, *Environ. Toxicol. Pharmacol.*, 16, 37–44 (2004).
 119. QSAR study using topological indices for inhibition of carbonic anhydrase II by sulfanilamides and Schiff bases. A. T. Balaban, S. C. Basak, A. Beteringhe, D. Mills, C. T. Supuran, *Mol. Diversity*, 8, 401–412 (2004).
 120. Similarity study of proteomic maps, Vracko, M., Basak, S. C., *Chemometr. Intell. Lab. Syst.*, 70, 33–38 (2004).
 121. Structure-mutagenicity modeling using counter propagation neural networks, M. Vracko, D. Mills, and S. C. Basak, *Environ. Toxicol. Pharmacol.*, 16, 25–36 (2004).
 122. Usefulness of graphical invariants in quantitative structure-activity correlations of tuberculostatic drugs of isonicotinic acid hydrazide type, Bagchi, M. C. Maiti, B. C. Mills, D. Basak, S. C., *J. Mol. Modeling*, 10, 102–111 (2004).
 123. Variable connectivity index as a tool for modeling structure-property relationships, M. Randić, M. Pompe, D. Mills, and S. C. Basak, *Molecules*, 9, 1177–1193 (2004), <http://www.mdpi.org/>.

124. Canonical labeling of proteome maps. Randić, M.; Lers, N.; Vukicević, D.; Plavšić, D.; Gute, B. D.; Basak, S. C., *J. Proteom. Res.*, 4, 1347–1352 (2005).
125. Chirality index, molecular overlay and biological activity of diastereoisomeric mosquito repellents, Natarajan, R.; Basak, S. C.; Balaban, A. T.; Klun, J. A.; Schmidt, W. F. *Pest. Manag. Sci.*, 61, 1193–1201 (2005).
126. Development of quantitative structure-activity relationship models for vapor pressure estimation using computed molecular descriptors, S. C. Basak, D. Mills, *ARKIVOC*, 10, 308–320 (2005), <http://www.arkat-usa.org/>.
127. Four-color map representation of DNA or RNA sequences and their numerical characterization, M. Randić, N. Lers, D. Plavšić, S. C. Basak, and A. T. Balaban, *Chem. Phys. Lett.*, 407, 205–208 (2005).
128. Information-theoretic biodescriptors for proteomics maps: Development and applications in predictive toxicology, S. C. Basak, B. D. Gute, F. Witzmann, Conference proceedings, *WSEAS Transactions on Information Science and Applications*, 7, 996–1001 (2005).
129. Predicting permeability of antimycotics from calculated chemodescriptors: A hierarchical QSAR approach, S. C. Basak and D. Mills, Conference proceedings, *WSEAS Transactions on Information Science and Applications*, 7, 954–957 (2005).
130. Prediction of partitioning properties for environmental pollutants using mathematical structural descriptors, S. C. Basak, D. Mills, *ARKIVOC, Part (ii)*, 10, 60–76 (2005), <http://www.arkat-usa.org/>.
131. Quantitative structure-activity modeling of *insect* juvenile hormone activity of 2,4-dienoates using computed molecular descriptors, Basak, S. C.; Natarajan, R.; Mills, D.; Hawkins, D. M.; Kraker, J. J., *SAR QSAR Environ. Res.*, 16, 581–606 (2005).
132. Structure-activity relationships for mosquito repellent aminoamides using the hierarchical QSAR method based on calculated molecular descriptors, S. C. Basak, R. Natarajan, D. Mills, Conference proceedings, *WSEAS Transactions on Information Science and Applications*, 7, 958–963 (2005).
133. Combining chemodescriptors and biodescriptors in quantitative structure-activity relationship modeling, Hawkins, D. M.; Basak, S. C.; Kraker, J. J.; Geiss, K. T.; Witzmann, F. A. *J. Chem. Inf. Model.*, 46, 9–16 (2006).
134. Complex graph matrix representations and characterizations of proteomic maps and chemically induced changes to proteomes. Balasubramanian, K.; Khokhani, K.; Basak, S. C. *Proteome Res.*, 5, 1133–1142 (2006).
135. Complexity of chemical graphs in terms of size, branching, and cyclicity. Balaban, A. T.; Mills, D.; Kodali, V.; Basak, S. C. *SAR QSAR Environ. Res.*, 17, 429–450 (2006).
136. On the dependence of a characterization of proteomics maps on the number of protein spots considered, Randić, M.; Witzmann, F. A.; Kodali, V.; Basak, S. C., *J. Chem. Inf. Model.*, 46, 116–122 (2006).
137. Optimal neighbor selection in molecular similarity: comparison of arbitrary versus tailored prediction spaces, Gute, B. D.; Basak, S. C. *SAR QSAR Environ. Res.*, 17, 37–51 (2006).
138. Prediction of tissue:air partition coefficients—Theoretical versus experimental methods, Basak, S. C.; Mills, D.; Gute, B. D., *SAR QSAR Environ. Res.*, 17, 515–532 (2006).
139. Proteomics maps-toxicity relationship of halocarbons studied with similarity index and genetic algorithm, Vracko, M.; Basak, S. C.; Geiss, K.; Witzmann, F. *J. Chem. Inf. Model.*, 46, 130–136 (2006).
140. Quantitative structure-activity relationship modeling of juvenile hormone mimetic compounds for *Culex pipiens Larvae*—with discussion of descriptor thinning methods, Basak, S. C.; Natarajan, R.; Mills, D.; Hawkins, D. M.; Kraker, J. J., *J. Chem. Inf. Model.*, 46, 65–77 (2006).
141. Statistical theory of spectra: Statistical moments as descriptors in the theory of molecular similarity. Bielinska-Waz, D.; Waz, P.; Basak, S. C. *Eur. Phys. J. B.*, 50, 333–338 (2006).
142. Graphical representation and numerical characterization of H5N1 avian flu neuraminidase gene sequence. Nandy, A.; Basak, S. C.; Gute, B. D. *J. Chem. Inf. Model.*, 47, 945–951 (2007).
143. A novel approach for the numerical characterization of molecular chirality. Natarajan, R.; Basak, S. C.; Neumann, T. *J. Chem. Inf. Model.*, 47, 771–775 (2007).
144. Quantitative structure-activity relationship (QSAR) modeling of juvenile hormone activity:

- Comparison of validation procedures, Kraker, J. J.; Hawkins, D. M.; Basak, S. C.; Natarajan, R.; Mills, D. *Chemometr. Intell. Lab. Syst.*, 87, 33–42 (2007).
145. Quantitative structure-activity relationship (QSAR) studies of quinolone antibacterials against *M. fortuitum* and *M. smegmatis* using theoretical molecular descriptors. Bagchi, M. C.; Mills, D.; Basak, S. C. *J. Mol. Modeling*, 13, 111–120 (2007).
 146. A quantitative structure-activity relationship (QSAR) study of dermal absorption using theoretical molecular descriptors. Basak, S. C.; Mills, D.; Mumtaz, M. M. *SAR QSAR Environ. Res.*, 18, 45–55 (2007).
 147. Similarity studies using statistical and genetical methods. Bielinska-Waz, D.; Waz, P.; Basak, S.C. *J. Math. Chem.*, 42, 1003–1013 (2007).
 148. Three dimensional structure-activity relationships (3D-QSAR) for insect repellency of diastereoisomeric compounds: A hierarchical molecular overlay approach. Basak, S. C.; Natarajan, R.; Nowak, W.; Miszta, P.; Klun, J. A. *SAR QSAR Environ. Res.*, 18, 237–250 (2007).
 149. Development and application of molecular similarity methods using nonempirical parameters. Basak, S.C.; Gute, B.D.; Grunwald, G.D. *Mathl. Model. Sci. Comput.*, in press.
 150. Quantitative comparison of five molecular structure spaces in selecting analogs of chemicals. Basak, S.C.; Gute, B.D.; Grunwald, G.D. *Mathl. Model. Sci. Comput.*, in press.
 151. Statistical spectroscopy as a tool for the study of molecular similarity. Bielinska-Waz, D.; Nowak, W.; Peplowski, L.; Waz, P.; Basak, S.C.; Natarajan, R. *J. Math. Chem.*, in press.
 152. Information-theoretic biodescriptors for proteomics maps: Application to rodent hepatotoxicity. Basak, S.C.; Gute, B.D.; Geiss, K.T.; Witzmann, F.A. *American Institute of Physics Conference Proceedings*, submitted.
 153. NMR spectral invariants — A new class of descriptors for diastereomers and enantiomers. Natarajan, R.; Basak, S. C. *Croat. Chem. Acta*, submitted.
 154. Proper statistical modeling and validation in QSAR: A case study in the prediction of rat fat-air partitioning, Basak, S.C.; Mills, D.; Hawkins, D.M.; Kraker, J.J. *American Institute of Physics Conference Proceedings*, submitted.
 155. Quantitative comparison of five molecular structure spaces in selecting analogs of chemicals. Basak, S.C.; Gute, B.D.; Grunwald, G.D. *American Institute of Physics Conference Proceedings*, submitted.
 156. Quantitative structure-activity relationship (QSAR) modeling of human blood:air partitioning with proper statistical methods and validation. S. C. Basak, D. Mills, D. M. Hawkins, and J. J. Kraker, *Drug Metab. Lett.*, submitted.
 157. Quantitative structure-activity relationship modeling of mosquito repellents using calculated descriptors. Natarajan, R.; Basak, S. C.; Mills, D.; Kraker, J. J.; Hawkins, D. M. *Croat. Chem. Acta*, submitted.

D. Review articles (4 total)

158. Use of molecular complexity indices in predictive pharmacology and toxicology: A QSAR approach, S.C. Basak, *Med. Sci. Res.*, 15, 605–609 (1987).
159. Understanding the molecular basis of Ayurvedic medicine: from structure-activity relationship (SAR) to composition-activity relationship (CAR), *aadi Katha* (1997).
160. Mathematical descriptors of DNA sequences: Development and application, Nandy, A.; Harle, M.; Basak, S. C. *ARKIVOC*, 9, 211–238 (2006).
161. Similarity methods in analog selection, property estimation and clustering of diverse chemicals. Basak, S. C.; Gute, B. D.; Mills, D. *ARKIVOC*, 9, 157–210 (2006).

E. Book chapters (30 total)

162. Information-theoretic topological indices of a molecular graph and their applications in QSAR, A.B. Roy, C. Raychaudhury, S.K. Ray, S.C. Basak, and J.J. Ghosh, *Proceedings of the Fourth European Symposium on Chemical Structure-biological Activity: Quantitative Approaches*, Elsevier, pp. 75–76 (1983).

163. Topological indices based on neighborhood symmetry: Chemical and biological applications, V.R. Magnuson, D.K. Harriss, and S.C. Basak, in *Chemical Applications of Topology and Graph Theory*, R.B. King, Ed., Elsevier, pp. 178–191 (1983).
164. Neighborhood complexities and symmetry of chemical graphs and their biological applications, A.B. Roy, S.C. Basak, D.K. Harriss, and V.R. Magnuson, in *Mathematical Modelling in Science and Technology*, X.J.R. Avula, R.E. Kalman, A.I. Liapis, and E.Y. Rodin, Eds., Pergamon Press, pp. 745–750 (1984).
165. A theoretical and computational approach to chemical evaluation based on structure-activity relationships, G.J. Niemi, S.C. Basak, and G.D. Veith, *Proceedings of the First conference of the International Society of Environmental Protection*, K. Zirm and J. Mayer, Eds., Federal Environmental Protection Agency, Vienna, WB. Druck Bmgh and Co, Reiden, Austria, pp. 57–68, volume 2 (1989).
166. A nonempirical approach to predicting molecular properties using graph-theoretic invariants, S.C. Basak, in *Practical Applications of Quantitative Structure-activity Relationships (QSAR) in Environmental Chemistry and Toxicology*, W. Karcher and J. Devillers, Eds., Kluwer Academic Publishers, pp. 83–103 (1990).
167. Recent developments in the characterization of chemical structure using graph-theoretic indices, S.C. Basak, G.J. Niemi, and G.D. Veith, in *Computational Chemical Graph Theory*, D.H. Rouvray, Ed., pp. 235–277, NOVA (1990).
168. Topological indices and chemical reactivity, O. Mekenyan, and S.C. Basak, in *Graph Theoretic Approaches to Chemical Reactivity*, D. Bonchev, and O. Mekenyan, Eds., Kluwer Academic Publishers, the Netherlands, pp. 221–239 (1994).
169. Predicting genotoxicity of chemicals using nonempirical parameters, S.C. Basak and G.D. Grunwald, in *Proceeding of XVI International Cancer Congress*, pp. 413–416 (1995).
170. Use of graph-theoretic and geometrical molecular descriptors in structure-activity relationships, S.C. Basak, G.D. Grunwald, and G.J. Niemi, in *From Chemical Topology to Three-dimensional Geometry*, Balaban, Ed., Plenum Press, New York, pp. 73–116 (1997).
171. Use of graph theoretic parameters in predicting inhibition of microsomal hydroxylation of anilines by alcohols: a molecular similarity approach, S.C. Basak and B.D. Gute, in *Proceedings of the International Congress on Hazardous Waste: Impact on Human and Ecological Health*, B.L. Johnson, C. Xintaras, and J.S. Andrews, Eds., Princeton Scientific Publishing Co, Inc, pp. 492–504, (1997).
172. Characterization of the molecular similarity of chemicals using topological invariants, S.C. Basak, B.D. Gute, and G.D. Grunwald, in *Advances in Molecular Similarity*, Ramon Carbo-Dorca and Paul G. Mezey, Eds., pp. 171–185, volume 2, JAI Press, Stanford, Connecticut (1998).
173. Relative effectiveness of topological, geometrical, and quantum chemical parameters in estimating mutagenicity of chemicals, S.C. Basak, B.D. Gute, and G.D. Grunwald, in *Quantitative Structure-activity Relationships in Environmental Sciences VII*, F. Chen and G. Schuurmann, Eds, SETAC Press, Pensacola, FL., pp. 245–261 (1998).
174. A hierarchical approach to the development of QSAR models using topological, geometrical and quantum chemical parameters, S.C. Basak, B.D. Gute, and G.D. Grunwald, in *Topological Indices and Related Descriptors in QSAR and QSPR*, J. Devillers and A.T. Balaban, Eds., Gordon and Breach Science Publishers, The Netherlands, pp. 675–696 (1999).
175. Information theoretic indices of neighborhood complexity and their applications, S.C. Basak, in *Topological Indices and Related Descriptors in QSAR and QSPR*, J. Devillers and A.T. Balaban, Eds., Gordon and Breach Science Publishers, The Netherlands, pp. 563–593 (1999).
176. Use of graph invariants in QMSA and predictive toxicology, S.C. Basak, B.D. Gute, and G. D. Grunwald, in *Discrete Mathematical Chemistry*, P. Hansen, P. Fowler, M. Zheng, Eds., DIMACS Series 51, American Mathematical Society: Providence, Rhode Island, pp. 9–24 (2000).
177. Modeling the solubility of aliphatic alcohols in water. Graph connectivity indices versus line graph connectivity indices, S. Nikolic, N. Trinajstic, D. Amic, D. Beslo, and S.C. Basak, in *QSAR/QSPR Studies by Molecular Descriptors*, M.V. Diudea, Ed., Nova Science Publishers, Huntington, New York, USA, pp. 63–81 (2001).
178. Applications of topological indices in the property/ bioactivity/ toxicity prediction of chemicals, S. C.

- Basak, D. Mills, B. D. Gute, G. D. Grunwald, and A. T. Balaban, in *Topology in Chemistry: Discrete Mathematics of Molecules*, D. H. Rouvray and R. B. King, Eds., Horwood Publishing Limited, Chichester, England, pp. 113–184 (2002).
179. Predicting mutagenicity of congeneric and diverse sets of chemicals using computed molecular descriptors: A hierarchical approach, S. C. Basak, D. Mills, B. D. Gute, and D. M. Hawkins, in *Quantitative Structure-Activity Relationship (QSAR) Models of Mutagens and Carcinogens*, R. Benigni, Ed., CRC Press, Boca Raton, FL, Chapter 7, pp. 207–234 (2003).
 180. Modeling of aryl hydrocarbon (Ah) receptor binding affinity for dibenzofurans using the hierarchical quantitative structure-activity relationship (HiQSAR) approach, Proceedings of the 2nd International Conference on the Chemistry and Biological Activity of Synthetic and Natural Compounds (CBC 2003), S. C. Basak and D. Mills, In *Oxygen- and Sulfur-Containing Heterocycles, Vol. 1*, V. G. Karstev, Ed.; IBS Press: Moscow, pp. 168 (2003).
 181. Predicting pharmacological and toxicological activity of heterocyclic compounds using QSAR and molecular modeling, S.C. Basak, D. Mills, B.D. Gute, and R. Natarajan, in *Topics in Heterocyclic Chemistry Vol. 5: QSAR and Molecular Modeling Studies of Heterocyclic Drugs*, S.P. Gupta, Ed., Springer-Verlag: Berlin-Heidelberg-New York, pp. 39–80 (2006).
 182. Quantitative structure-toxicity relationships using chemodescriptors and biodescriptors, S.C. Basak, D. Mills, and B.D. Gute, in *Biological Concepts and Techniques in Toxicology: An Integrated Approach*, J.E. Riviere, Ed., Taylor & Francis, New York, pp. 61–82 (2006).
 183. Statistical theory of spectra as a tool in molecular similarity, D. Bielinska-Waz, P. Waz, S.C. Basak, and R. Natarajan, in *Symmetry, Spectroscopy, and SCHUR*, R.C. King, Ed., Nicolaus Copernicus University Press: Torun, pp. 27–32 (2006).
 184. Predicting bioactivity and toxicity of chemicals from mathematical descriptors: A chemical-cum-biochemical approach, S.C. Basak, D. Mills, and B.D. Gute, in *Advances in Quantum Chemistry*, D.J. Klein, E. Brandas, Eds., Elsevier, in press.
 185. Use of mathematical structural invariants in analyzing combinatorial libraries: A case study with Psoralen derivatives, S.C. Basak, D. Mills, B.D. Gute, A.T. Balaban, K. Basak, and G.D. Grunwald, in *Some Aspects of Mathematical Chemistry*, D.K. Sinha, S.C. Basak, R.K. Mohanty and I.N. Basumallick, Eds., Visva-Bharati University, India, in press.
 186. Use of proteomics based biodescriptors in the characterization of chemical toxicity, Z. Bajzer, S.C. Basak, M. Vracko, and M. Randic, in *Genomic and Proteomic Applications to Toxicity Testing*, M.J. Cunningham, Ed., in press.
 187. Variable molecular descriptors, M. Randic and S.C. Basak, in *Some Aspects of Mathematical Chemistry*, D.K. Sinha, S.C. Basak, R.K. Mohanty and I.N. Basumallick, Eds., Visva-Bharati University, India, in press.
 188. Molecular overlay as a tool to model bio-specificity: A case study with mosquito repellents, R. Natarajan and S.C. Basak, in *Lecture Notes of the First Indo-US Lecture Series on Discrete Mathematical Chemistry*, S. C. Basak and R. Balakrishnan, Eds., submitted.
 189. Molecular similarity: Defining, quantifying and tailoring structure spaces, B.D. Gute and S.C. Basak, in *Lecture Notes of the First Indo-US Lecture Series on Discrete Mathematical Chemistry*, S. C. Basak and R. Balakrishnan, Eds., submitted.
 190. Use of graph invariants in the protection of human and ecological health, S.C. Basak, D. Mills, and M.M. Mumtaz, in *Lecture Notes of the First Indo-US Lecture Series on Discrete Mathematical Chemistry*, S. C. Basak and R. Balakrishnan, Eds., submitted.
 191. Characterization of toxicoproteomics maps for mixtures and individual toxicants using information theoretic approach, S.C. Basak, B.D. Gute, N.A. Monteiro-Riviere, and F.A. Witzmann, in *Principles and Practice of Mixture Toxicity*, M.M. Mumtaz, Ed., Wiley-VCH Weinheim, submitted.

F. Extended Abstracts (8 total)

192. Chemistry *in silico* as a tool for hazard assessment and drug discovery: Prospects and problems, S.C. Basak, D. Mills, B. D. Gute, and G. D. Grunwald, in Book of Abstracts, CIMA 2001 (International ICSC Congress on Computational Intelligence: Methods and Applications), June 19–22, 2001,

University of Wales, Bangor.

193. Use of statistical and neural net methods in predicting toxicity of chemicals: A hierarchical QSAR approach, S.C. Basak, B.D. Gute, G. D. Grunwald, and D. Opitz, in American Association of Artificial Intelligence conference, Predictive Toxicology of Chemicals: Experiences and Impact of AI Tools, Stanford University, 1999.
194. Hazard assessment modeling: A hierarchical QSAR approach. International Conference on Artificial Intelligence and Soft Computing, D. Opitz and S. Basak, 2000.
195. A comparative study of arbitrary versus tailored molecular similarity metrics in property / toxicity / bioactivity prediction, S.C. Basak and B.D. Gute, in *Lecture Series on Computer and Computational Sciences, Vol. 3*, Brill Academic Publishers: The Netherlands, 2005.
196. Use of proteomics based biodescriptors versus chemodescriptors in predicting halocarbon toxicity: An integrated approach, S.C. Basak, in *Lecture Series on Computer and Computational Sciences, Vol. 3*, Brill Academic Publishers: The Netherlands, 2005.
197. Molecular similarity metrics in property prediction, B.D. Gute and S.C. Basak, in *Lecture Notes for the 2ND Indo-US Lecture Series on Discrete Mathematical Chemistry*, June 20–25, Kalpetta, Kerala, India, 2007.
198. Mathematical structure descriptors: Development and applications in chemistry, drug discovery, environmental protection, and bioinformatics, S.C. Basak, in *Lecture Notes for the 2ND Indo-US Lecture Series on Discrete Mathematical Chemistry*, June 20–25, Kalpetta, Kerala, India, 2007.
199. Numerical characterization of molecular chirality, R. Natarajan and S.C. Basak, in *Lecture Notes for the 2ND Indo-US Lecture Series on Discrete Mathematical Chemistry*, June 20–25, Kalpetta, Kerala, India, 2007.

G. Editorials and Popular Articles (4 total)

200. 1st Indo-US Workshop on Mathematical Chemistry, Editorial, S.C. Basak, G.W.A. Milne, M. Randic, D.K. Sinha, *J. Chem. Inf. Comput. Sci.*, 39, 179 (1999).
201. 2nd Indo-US Workshop on Mathematical Chemistry, Editorial, S.C. Basak, G.W.A. Milne, M. Randic, D.K. Sinha, *J. Chem. Inf. Comput. Sci.*, 41, 479 (2001).
202. My tortuous journey from biochemistry to mathematical chemistry, S. C. Basak, in *Proceedings of the 60th Anniversary of the Department of Biochemistry*, University of Calcutta, Kolkata, India (2005).
203. 4th Indo-US Workshop on Mathematical Chemistry, Editorial, D.K. Sinha, S.C. Basak, *J. Chem. Inf. Model.*, 46, 1 (2006).

Technical Reports

1. Report of the International Workshop “Molecular similarity and risk assessment” to USEPA, submitted by Subhash Basak (PI), Bob Hunter, Gerald Niemi and George Host, Technical Report No. NRRI/TR-93/09 (8/93).
2. Stereo-electronic factors in molecular similarity and risk assessment, Technical report No. NRRI/TR-94/93, submitted to USEPA by Subhash Basak (PI), Bob Hunter, Gerald Niemi and George Host (Co-PIs) (8/93).
3. Annual Progress Report of the USEPA project “Computational techniques to quantify chemical similarity: tools for risk assessment, Technical Report No. NRRI/TR-93-26, by Subhash Basak (PI), Bob Hunter, Gerald Niemi and George Host (Co-PIs) (8/93).
4. Final Transition Documentation Report of the NIH contract “Structure-activity relationships for anticonvulsant drug development”- Technical System Documentation- submitted to NIH by Subhash Basak (PI) (6/94).
5. Final Transition Documentation Report of the NIH contract “Structure-activity relationships for anticonvulsant drug development”- User Documentation- submitted to NIH by Subhash Basak (PI) (6/94).
6. Quarterly Report # 3.4 of the NIH contract “Structure-activity relationships for anti convulsant drug development” submitted to NIH by Subhash Basak (PI) (9/94).
7. Final Report of the USEPA project “Computational techniques to quantify chemical similarity: tools for risk assessment, Technical Report No. NRRI/TR-95/30 (7/95).
8. Annual Technical Report of the structure-activity consortium project “Predicting environmental toxicity of

- chemicals using molecular similarity,” submitted to the Exxon Corporation by Subhash Basak (PI) and Gerald Niemi (Co-PI), Technical Report No. NRRI/TR-95/02 (1/96).
9. Progress Report of the US Air Force project “Predicting toxicity and degradability of quadricyclane, fluorocarbon ethers and their analogs,” submitted by Subhash Basak (PI), Keith Lodge and Joseph Schubauer-Berigan (Co-PIs), Technical Report No. NRRI/TR-96/14 (8/96).
 10. Progress Report of the US Air Force project “Predicting toxicity and degradability of quadricyclane, fluorocarbon ethers and their analogs,” submitted by Subhash Basak (PI), Keith Lodge and Joseph Schubauer-Berigan (Co-PIs), Technical Report No. NRRI/TR-97/15 (8/97).
 11. Progress Report of the Air Force AASERT project “Quantitative characterization of molecular similarity spaces: tools for computational toxicology,” submitted by Subhash Basak (PI) to Air Force Office of Scientific Research, Technical Report No. NRRI/TR-97/16 (8/97).
 12. Final Technical Report of the US Air Force project “Predicting toxicity and degradability of quadricyclane, fluorocarbon ethers and their analogs,” submitted by Subhash Basak (PI), Keith Lodge and Joseph Schubauer-Berigan (Co-PIs), Technical Report No. NRRI/TR-97/15a (10/97).
 13. Progress Report of the Air Force AASERT project “Quantitative characterization of molecular similarity spaces: tools for computational toxicology,” submitted by Subhash Basak (PI) to Air Force Office of Scientific Research, Technical Report No. NRRI/TR-98/15 (8/98).
 14. Progress Report of the US Air Force project “Prediction of health and environmental hazards of chemicals: A hierarchical approach using QMSA and QSAR,” submitted by Subhash Basak (PI) to Air Force Office of Scientific Research, Technical Report No. NRRI/TR-98/14 (8/98).
 15. Progress Report of the US Air Force project “Prediction of health and environmental hazards of chemicals: A hierarchical approach using QMSA and QSAR,” submitted by Subhash Basak (PI) to Air Force Office of Scientific Research, Technical Report No. NRRI/TR-99/13 (8/99).
 16. Progress Report of the Air Force AASERT project “Quantitative characterization of molecular similarity spaces: tools for computational toxicology,” submitted by Subhash Basak (PI) to Air Force Office of Scientific Research, Technical Report No. NRRI/TR-99/14 (8/99).
 17. Final Technical Report of the Air Force AASERT project “Quantitative characterization of molecular similarity spaces: tools for computational toxicology,” submitted by Subhash Basak (PI) to Air Force Office of Scientific Research, Technical Report No. NRRI/TR-2000/02 (1/00).
 18. Final Technical Report of the US Air Force project “Prediction of health and environmental hazards of chemicals: A hierarchical approach using QMSA and QSAR,” submitted by Subhash Basak (PI) to Air Force Office of Scientific Research, Technical Report No. NRRI/TR-2000/44 (10/00).
 19. Progress Report of the US Air Force project “Integration of biodescriptors and chemodescriptors for predictive toxicology: A mathematical / computational approach,” submitted by Subhash Basak (PI) to Air Force Office of Scientific Research, Technical Report No. NRRI/TR-2001/27 (8/01).
 20. Progress Report of the US Air Force project “Use of biodescriptors and chemodescriptors in predictive toxicology: A mathematical / computational approach,” submitted by Subhash Basak (PI) to Air Force Office of Scientific Research, Technical Report No. NRRI/TR-2002/12 (8/02).
 21. Progress Report of the US Air Force project “Use of biodescriptors and chemodescriptors in predictive toxicology: A mathematical / computational approach,” submitted by Subhash Basak (PI) to Air Force Office of Scientific Research, Technical Report No. NRRI/TR-2003/20 (8/03).
 22. Progress Report of the US Air Force project “Use of biodescriptors and chemodescriptors in predictive toxicology: A mathematical / computational approach,” submitted by Subhash Basak (PI) to Air Force Office of Scientific Research, Technical Report No. NRRI/TR-2004/22 (8/04).
 23. Final Report of the US Air Force project “Use of biodescriptors and chemodescriptors in predictive toxicology: A mathematical / computational approach,” submitted by Subhash Basak (PI) to Air Force Office of Scientific Research, Technical Report No. NRRI/TR-2005/13 (5/05).
 24. Progress Report of the US Air Force project “Predicting chemical toxicity from proteomics and computational chemistry,” submitted by Subhash Basak (PI) to Air Force Office of Scientific Research, Technical Report No. NRRI/TR-2006/20 (8/06).
 25. Progress Report of the US Air Force project “Predicting chemical toxicity from proteomics and computational

chemistry,” submitted by Subhash Basak (PI) to Air Force Office of Scientific Research, Technical Report No. NRRI/TR-2007/21 (8/07).

Development of software

Led the development of the following software pertinent to QSAR and molecular modeling:

1. *POLLY*, a computer program written in Pascal, is capable of calculating some ninety topological indices for molecules.
2. *GENETOX.CAN*, a computer program written in MINTER, is capable of classifying and predicting genotoxic potential of chemicals.
3. *TICPAC*, a computer software capable of calculating octanol-water partition coefficient (Kow) of chemicals directly from structure.
4. *APPROBE*, a software capable of generating atom pairs from the chemical graphs of molecules.
5. *H-BOND*, a software capable of calculating hydrogen bonding ability of molecules.

Molecular design and drug discovery

1. Designed and synthesized six antiepileptic compounds using computer assisted drug design methodology (patent to be applied for), in collaboration with Alexandru T. Balaban.
2. Designed a number of anti diabetic drugs which are currently being tested (patent to be applied for), in collaboration with Alexandru T. Balaban.
3. Designed a series of effective and less toxic deicing agents using computational methods.

Patent Activity

1. New methods for obtaining styrylpyridinium or styryl-isobenzopyrylium compounds: structure-photoactivity relationships, A.T. Balaban and S.C. Basak (pending) 2000.

Professional activities

A. Advisory positions

1. Member, International Committee, International Association for Mathematical and Computer Modelling.
2. Member, Organizing Committee, QSAR '92.
3. Principal Reviewer: Peer Review Workshop on Cancer Expert System, US EPA, 1992.
4. Organizer, First Indo-US Workshop on Mathematical Chemistry, West Bengal India, Jan 9–13, 1998.
5. Organizer, Symposium on Applied Mathematical Chemistry, Natural Resources Research Institute, University of Minnesota–Duluth, May 3, 1999.
6. Organizer, Second Indo-US Workshop on Mathematical Chemistry, Duluth, Minnesota, May 30–June 3, 2000.
7. Member, Indian National Organizing Committee of the International Symposium “Strategies and Perspectives in Drug Development, Design and Molecular Modelling,” organized by the Indian Institute of Chemical Biology, Calcutta, India, Oct 17–18, 2000.
8. Member of the International Advisory Committee, International Symposium of Current Trends in Drug Discovery Research, Central Drug Research Institute, Lucknow, India, Feb 11–15, 2001.
9. Organizer, Third Indo-US Workshop on Mathematical Chemistry, Duluth, Minnesota, August 2–7, 2003.
10. Organizer, Fourth Indo-US Workshop on Mathematical Chemistry, Pune, Maharashtra, India, January 8–12, 2005.
11. Organizer, international conference on Drug Discovery Based on Darjeeling Area Biodiversity, November 7, 2005.
12. Organizer, mini-symposium at a conference on Current Advances in QSAR Studies in Kolkata, India, November 8, 2005.

13. Organizer, First Indo-US Lecture Series on Discrete Mathematical Chemistry, Bangalore, India, January 8–11, 2007.
14. Organizer, Second Indo-US Lecture Series on Discrete Mathematical Chemistry, Kalpetta, Kerala, India, June 20–25, 2007.
15. Member of the International Scientific Advisory Board, Fourth International Symposium on Computational Methods in Toxicology and Pharmacology Integrating Internet Resources, Moscow, Russia, Sep 1–5, 2007.
16. Organizer, Third Indo-US Lecture Series on Discrete Mathematical Chemistry, Tiruchirappalli, Tamil Nadu, India, January 7–11, 2008.
17. Organizer, Fifth Indo-US Workshop on Mathematical Chemistry, Duluth, Minnesota, June 2008.

B. Symposia and workshops

1. Target enzyme desensitization following multiple sumithion administration, R. Sengupta, S.C. Basak, D. Sarkar, and J.J. Ghosh, paper presented at the *International Symposium on Oriental Entomology*, Calcutta, India (1976).
2. A mathematical model for drug tolerance, S.C. Basak, A.B. Roy, and J.J. Ghosh, *International Symposium and Workshop on Biomedical Engineering*, New Delhi, India (1978).
3. Information-theoretic studies on the pharmacological action of drugs, S.C. Basak, B. Dutta, A.B. Roy, and J.J. Ghosh, Proceeding to the *Seventh All-India Biomedical Engineering Symposium*, Hyderabad, India (1978).
4. Information theoretic analysis of structure-activity relationship of drugs, S.C. Basak, B. Dutta, C. Sarkar, A.B. Roy, and J.J. Ghosh, Abstract: Second National Conference, Forum for Interdisciplinary Mathematics, Jaipur, India (1978).
5. A study of the relationship of physicochemical and pharmacological properties of drug molecules with their structural information. S.C. Basak, C. Sarkar, S. Mukherjee, A.B. Roy, and J.J. Ghosh, paper presented at the Annual Convention of Chemists, Waltair, India (1978).
6. Some aspects of electro-acupuncture treatment: its possible clinical implication, S. Das, A. Ganguly, S.C. Basak, P. Banerjee, T.K. Chattered, and J.J. Ghosh, paper presented at the First All India Conference on Acupuncture.
7. A comparative study of molecular connectivity and hydrophobicity in the quantitative correlation of antifungal properties of substituted phenols, A.K. Samanta, S.K. Ray, S.C. Basak, and S.K. Bose, Proceedings of the Indian Convention of Chemists, Madras, India, 1981.
8. Bonding information content (BIC): a new parameter for QSAR study, S.K. Ray, S.C. Basak, C. Raychaudhury, J.J. Ghosh, and A.B. Roy, Proceedings of the Indian Conventional of Chemists, Madras, India (1981).
9. Molecular topology and biological function: a quantitative structure-activity relationship study of barbiturates using bonding information content (BIC), S.K. Ray, S.C. Basak, C. Raychaudhury, J.J. Ghosh, and A.B. Roy, paper presented at the All-India Symposium on Biological Sciences and Engineering, Calcutta, India (1981).
10. Graph-theoretical invariant and thermodynamic property: a QSAR study of alcohols, C. Raychaudhury, S.C. Basak, S.K. Ray, A.B. Roy, and J.J. Ghosh, presented at the Nineteenth Annual Meeting, Society of Engineering Sciences, Inc, University of Missouri-Rolla, Missouri (1982).
11. Topological indices based on neighborhood symmetry and their applications, V.R. Magnuson, D.K. Harriss, and S.C. Basak, paper presented at the Seventeenth Great Lakes Regional Meeting of American Chemical Society, College of St Catherine, St Paul, MN (1983).
12. A computerized rule-based system for the prediction of carcinogenicity of chemicals, S.C. Basak, V.R. Magnuson, G.J. Niemi, and G.D. Veith, presented at the Eight Annual Meeting, Society of Environmental Toxicology and Chemistry, Pensacola, FL (1987).
13. Recent developments in the characterization of chemical structure, S.C. Basak, G.J. Niemi, and G.D. Veith, paper presented in the symposium entitled “Computational Graph Theory and Combinatorics” at

- the 196th Annual Meeting of the American Chemical Society, Sept 25–30, 1988, Los Angeles (1988).
14. Predicting physicochemical and environmental properties of chemicals from their topological invariants, S.C. Basak and G.J. Niemi, presented at the 32nd Conference on Great Lakes Research, Madison, WI (1989).
 15. Molecular similarity analysis, S.C. Basak, presented at the Peer Review of Research Programs of the environmental Research Laboratory, Duluth, Minnesota (1989).
 16. A graph-theoretic approach to predicting molecular properties, S.C. Basak, G.J. Niemi, and G.D. Veith, presented at the Seventh International Conference on Mathematical and Computer Modelling, Chicago (1989).
 17. Use of graph-theoretic invariants in structure-activity studies, S.C. Basak and G.J. Niemi, presented at the symposium Progress in Mathematical Modelling in Chemistry of PACIFICHEM held December 17–22 in Honolulu (1989).
 18. A comparative study graph invariants, volume and total surface area in predicting boiling point of alkanes, SC Basak and GD Grunwald presented at the Eighth International Conference on Mathematical and Computer Modelling held April 1–4, University of Maryland, College Park, MD, (1991).
 19. Search for empirical descriptors and heteroatoms in QSAR, M. Randic and S.C. Basak, presented at the Eighth International Conference on Mathematical and Computer Modelling held April 1–4, University of Maryland, College Park, MD (1991).
 20. Application of graph theoretic parameters in quantifying molecular similarity and structure-activity studies, S.C. Basak, S. Bertelsen, and G. Grunwald, presented at the Fifth International Conference on Mathematical and Computational Chemistry, University of Missouri, Kansas, May 17–21, (1993).
 21. Use of topological indices and atom pairs in the quantification of molecular similarity, S.C. Basak and G. Grunwald, presented at the Ninth International Conference on Mathematical and Computer Modelling, University of California, Berkeley, July 26–29 (1993).
 22. Construction of optimal molecular descriptors for heteroatoms, M. Randic and S.C. Basak, presented at the Ninth International Conference on Mathematical and Computer Modelling, University of California, Berkeley (1993).
 23. Predicting mutagenicity of chemicals using topological and quantum chemical parameters, S.C. Basak, presented at the 207th Annual Meeting of the American Chemical Society, San Diego, CA, March 13–18 (1994).
 24. Use of graph invariants in predicting bioactivity of molecules, S.C. Basak and G.D. Grunwald, presented at the NATO Advanced Study Institute (ASI) Workshop on Pharmacokinetics, Erice Sicily April 4–16 (1994).
 25. Tolerance space and molecular similarity, S.C. Basak, presented at the Sixth International Workshop on Quantitative Structure-activity Relationships (QSAR) in Environmental Sciences, Belgirate, Italy, Sept 10–18 (1994).
 26. Predicting genotoxicity of chemicals using nonempirical parameters, S.C. Basak, presented at the Sixteenth International Cancer Congress, New Delhi, India, Oct 30–Nov 5 (1994).
 27. Use of graph theoretic parameters in predicting inhibition of microsomal p0hydroxylation of aniline by alcohols: a molecular similarity approach, S.C. Basak and B.D. Gute, presented at the International Congress on Hazardous Waste: Impact on Human and Ecological Health, Atlanta, GA June 5–8 (1995).
 28. Development and applications of molecular similarity methods using nonempirical parameters, S.C. Basak, G.D. Grunwald, and B.D. Gute, presented at the Tenth International Conference Mathematical and Computer Modelling and Scientific Computing, Boston MA July 5–8 (1995).
 29. Modelling mutagenicity with artificial neural networks, S.C. Basak, D. Axtell, and T. Colburn, presented at the Tenth International Conference of Mathematical and Computer Modelling and Scientific Computing, Boston, July 5–8 (1995).
 30. The relationship of topological, topochemical, and geometrical parameters in estimating environmental properties of chemicals, S.C. Basak, B.D. Gute, and G.D. Grunwald, presented at the Seventh

- International Workshop on QSARs in Environmental Sciences, Copenhagen, Denmark, June 22–29 (1996).
31. Development of QSARs of bioactive molecules using a hierarchical approach, B.D. Gute, G.D. Grunwald, and S.C. Basak, presented at the American Chemical Society 32st Midwest Regional Meeting, Sioux Falls, SD, Nov 6–8 (1996).
 32. "Dissimilarity-based clustering of psoralen derivatives in the topological structure space: a strategy for drug design" at the 'Second Annual Chemoinformatics Workshop', organized by the Cambridge Health Institute, Boston, MA, June 15–16, 1998.
 33. "Predicting mode of action of chemicals from structure: A hierarchical approach" presented at the International Conference Computational Methods in Toxicology held in Dayton, OH, April 20–22, 1998.
 34. "Use of computational methods in predicting potential toxicity of chemicals" presented at the International Conference Computational Methods in Toxicology held in Dayton, OH, April 20–22, 1998.
 35. "Dissimilarity-based clustering of psoralen derivatives in the topological structure space: A strategy for drug design" presented at the Second Annual Chemoinformatics Workshop, organized by the Cambridge Health Institute, Boston, MA, June 15–16, 1998.
 36. "A computational approach to predicting toxicity and toxic modes of action of chemicals from structure" presented at the International Conference Smarter Lead Optimization: Easing the Bottleneck organized by Cambridge Health Institute, San Diego, CA, March 18–19, 1999.
 37. "Use of statistical and neural net methods in predicting toxicity of chemicals: A hierarchical QSAR approach" presented at the American Association of Artificial Intelligence conference, Predictive Toxicology of Chemicals: Experiences and Impact of AI Tools, Stanford University, March 22–24, 1999.
 38. "A hierarchical QSAR approach for predicting property/activity of chemicals" presented at the QSAR Gordon Conference, Tilton, New Hampshire, July 25–30, 1999.
 39. "Clustering of Psoralen derivatives using topological invariants: A strategy for molecular design" presented at the 13th International Biophysics Congress, New Delhi, September of 1999.
 40. "A hierarchical QSAR approach to predicting bioactivity of chemicals using theoretical molecular descriptors" presented at the 13th International Biophysics Congress, New Delhi, September of 1999.
 41. "Modeling the solubility of aliphatic alcohols in water, graph connectivity indices versus line graph connectivity indices" presented at the 13th International Biophysics Congress, New Delhi, September of 1999.
 42. "Design of high quality structure-property regressions" presented at the 13th International Biophysics Congress, New Delhi, September of 1999.
 43. "On numerical characterization of DNA primary sequences" presented at the 13th International Biophysics Congress, New Delhi, September of 1999.
 44. "Clustering of JP-8 chemicals using structure spaces and property spaces: A computational approach" presented the International Conference on Medicinal Chemistry and Biocatalysis organized by Delhi University, India, January 26–29, 2000.
 45. "Prediction of gas chromatographic retention indices using variable connectivity index" presented the International Conference on Medicinal Chemistry and Biocatalysis organized by Delhi University, India, January 26–29, 2000.
 46. "Clustering of Psoralen derivatives using topological invariants: A strategy for molecular design" presented the International Conference on Medicinal Chemistry and Biocatalysis organized by Delhi University, India, January 26–29, 2000.
 47. "A novel structure-activity approach to benzamidines complement inhibitory activity" presented the International Conference on Medicinal Chemistry and Biocatalysis organized by Delhi University, India, January 26–29, 2000.
 48. "On the use of variable connectivity index for characterization of amino acids," presented at the 40th

- SANIBEL SYMPOSIUM on atomic, molecular, biophysical and condensed matter theory organized by the Quantum Theory Project, University of Florida, February 26–March 3, 2000.
49. “Estimating physicochemical and toxicological properties of chemicals from calculated molecular descriptors” presented at the Dept. of Energy’s Environmental Management Sciences Program National Workshop in Atlanta, April, 2000.
 50. “On the clustering of psoralens,” presented at the Second Indo-US Workshop on Mathematical Chemistry, organized jointly by NRRI/ UMD and Visva Bharati University, India, May 30–June 3, 2000.
 51. “Molecular similarity based estimation of properties: A comparison of structure spaces and property spaces,” presented at the Second Indo-US Workshop on Mathematical Chemistry, organized jointly by NRRI/ UMD and Visva Bharati University, India, May 30–June 3, 2000.
 52. “Molecular similarity based estimation of properties: A comparison of structure spaces and property spaces,” presented at the Second Indo-US Workshop on Mathematical Chemistry, organized jointly by NRRI/ UMD and Visva Bharati University, India, May 30–June 3, 2000.
 53. “Clustering of chemical using theoretical structure spaces: A case study with 476 diverse chemicals,” presented at the Second Indo-US Workshop on Mathematical Chemistry, organized jointly by NRRI/ UMD and Visva Bharati University, India, May 30–June 3, 2000.
 54. “Clustering of JP-8 chemicals using property spaces and structure spaces: A novel tool for hazard assessment,” presented at the Second Indo-US Workshop on Mathematical Chemistry, organized jointly by NRRI/ UMD and Visva Bharati University, India, May 30–June 3, 2000.
 55. “On use of the variable connectivity index in QSAR: Toxicity of aliphatic ethers,” presented at the Second Indo-US Workshop on Mathematical Chemistry, organized jointly by NRRI/ UMD and Visva Bharati University, India, May 30–June 3, 2000.
 56. “Topological indices as valuable molecular descriptors for QSAR and QSPR,” presented at the Second Indo-US Workshop on Mathematical Chemistry, organized jointly by NRRI/ UMD and Visva Bharati University, India, May 30–June 3, 2000.
 57. “Prediction of gas chromatographic retention indices for oxygenated compounds using variable connectivity index,” presented at the Second Indo-US Workshop on Mathematical Chemistry, organized jointly by NRRI/ UMD and Visva Bharati University, India, May 30–June 3, 2000.
 58. “Topological indices: Their nature and mutual relatedness,” presented at the Second Indo-US Workshop on Mathematical Chemistry, organized jointly by NRRI/ UMD and Visva Bharati University, India, May 30–June 3, 2000.
 59. “Predicting property/activity/toxicity of chemicals using calculated molecular descriptors” presented at the University of Florida, Gainesville, June 19, 2000.
 60. “Similarity-based estimation of properties: A comparison of structure spaces” presented at the American Chemical Society Annual meeting recently in Washington, D.C., August 20–24, 2000.
 61. “Trends and possibilities for future developments of topological indices,” presented at the American Chemical Society Annual meeting recently in Washington, D.C., August 20–24, 2000.
 62. “Use of graph invariants for the prediction of property/activity/toxicity of chemicals,” presented at the American Chemical Society Annual meeting recently in Washington, D.C., August 20–24, 2000.
 63. “Clustering of JP-8 chemicals using structure spaces and property spaces: A computational approach,” presented at the American Chemical Society Annual meeting recently in Washington, D.C., August 20–24, 2000.
 64. “Hierarchical clustering of Psoralen derivatives using topological invariants: A strategy for molecular design,” presented at the American Chemical Society Annual meeting recently in Washington, D.C., August 20–24, 2000.
 65. “Use of variable connectivity indices on biological molecules,” presented at the American Chemical Society Annual meeting recently in Washington, D.C., August 20–24, 2000.
 66. “Hazard Assessment Modeling: A Hierarchical QSAR Approach.” International Conference on Artificial Intelligence and Soft Computing, Opitz, D and Basak, S, 2000.

67. "Use of mathematical structural descriptors in predicting property/ activity of chemicals: A hierarchical approach," presented at Pacificchem 2000, Honolulu, Hawaii, December 14–19, 2000.
68. "A study of the intercorrelation of topological indices," presented at Pacificchem 2000, Honolulu, Hawaii, December 14–19, 2000.
69. "A comparison of five molecular similarity spaces," presented at Pacificchem 2000, Honolulu, Hawaii, December 14–19, 2000.
70. "Comparing structural spaces for similarity-based estimation of properties," presented at Pacificchem 2000, Honolulu, Hawaii, December 14–19, 2000.
71. "Hierarchical use of structural invariants in the clustering of a virtual Psoralen combinatorial library," presented at Pacificchem 2000, Honolulu, Hawaii, December 14–19, 2000.
72. "Use of variable molecular descriptors for the characterization of biological molecules," presented at Pacificchem 2000, Honolulu, Hawaii, December 14–19, 2000.
73. "On mathematical characterization of proteomics maps," presented at the international symposium Current Trends in Drug Design organized February 11–15, 2001, Lucknow, India.
74. "On the characterization of DNA primary sequences by triplet of nucleic acid bases," presented at the international symposium Current Trends in Drug Design organized February 11–15, 2001, Lucknow, India.
75. "Issues and applications in toxicology and risk assessment," organized jointly by the Food and Drug Administration (FDA), Agency for Toxic Substances and Disease Registry (ATSDR), Air Force Research Laboratory (AFRL), US Army, U S Environmental Protection Agency and the National Institute of Environmental Health Sciences (NIEHS) during April 23–26, 2001, Dayton, OH.
76. "Use of biodescriptors and chemodescriptors in predicting toxicity of chemicals: A mathematical-cum-computational approach," presented at the Air Force Office of Scientific Research Predictive Toxicology Review and Planning Workshop, Dayton, OH, May 15–16, 2001.

C. Invited participation in symposia and conferences

1. Third Society for Industrial and Applied Mathematics (SIAM) Conference on Discrete Mathematics, Clemson University, South Carolina, 1986. Presented "Some problems in characterization of structural similarity."
2. Sixth International Conference on Mathematical Modelling, Washington University, St Louis, MO, 1987. Presented "Topological indices: their nature and interrelatedness."
3. Tenth Annual Midwest Biopharmaceutical Statistics Workshop, Ball State University, Muncie, IN, 1987. Presented "An approach to drug design using topological similarity."
MAA Summer Seminar on Linear Algebra and Graph Theory, University of Minnesota Duluth, 1987. Presented "Prospective use of graph invariants in drug design and toxicological risk assessment."
4. Society of Environmental Toxicology and chemistry (SETAC) Annual Meeting, Alexandria, Virginia, 1988. Presented "A computerized system for the assessment of carcinogenicity of chemicals" in the session Carcinogenicity/Toxicity in Aquatic Species.
5. Delivered a lecture entitled, "A graph-theoretic approach to predicting molecular properties" at the EURO COURSES organized by the European Commission at Ispra, Italy, June (1990).
6. Joint Central Great Lakes Regional Meeting of the American Chemical Society, Indianapolis, 1991. Presented "Use of orthogonal nonempirical parameters in QSAR."
7. Presented "Use of graph theoretic parameters in risk assessment of chemical" at the International workshop entitled Decision Support Methodologies for Human Health Risk Assessment of Toxic Substances, Oct 18–20, 1993, in Atlanta, GA, under the auspices of US Department of Health and Human Services.
8. Presented "Predicting mutagenicity of chemicals using topological and quantum chemical parameters at the Environmental Chemistry Section of the 207th Annual Meeting of the American Chemical Society, San Diego, CA, Mar 12–18 (1994).
9. Presented "Predicting biomedical and environmental properties of chemicals using graph theoretic

- parameters” at the NATO Advanced Study Institute on pharmacokinetics, Erice, Sicily, April 6 (1994).
10. Presented “Tolerance space and molecular similarity” at the Sixth International Workshop on Quantitative Structure-activity Relationships (Qsar) in Environmental Sciences. Belgirate, Italy, Sept 10–18 (1994).
 11. Presented “Molecular similarity and estimation of molecular properties” at the Skolnick Award Symposium for Chemical Information, 308th Annual Meeting of the American Chemical Society, Washington DC, August 20–25 (1994).
 12. Presented “QSARs using topological, topochemical and geometrical parameters; a hierarchical approach,” at the Skolnick Award Symposium for Chemical Information 292th Annual Meeting of the American Chemical Society, Orlando FL, August 25–29 (1996).
 13. “Rational drug design and Ayurvedic medicine” presented at the conference organized by the Association of Ayurvedic Doctors of India (AADI) in India, January 4, 1998.
 14. “Use of computational methods and Ayurvedic knowledge in modern drug discovery” presented at the conference AYURVEDIA TODAY in India, January 8, 1998.
 15. “Graph invariants, molecular similarity and QSAR” presented at the First Indo/US Workshop on Mathematical Chemistry, organized jointly by NRRI and Visva Bharati University, Santiniketan, West Bengal India, Jan 9–13, 1998.
 16. “Dissimilarity based clustering of psoralen derivatives in the topological structure space: A strategy for drug design” presented at the First Indo/US Workshop on Mathematical Chemistry, organized jointly by NRRI and Visva Bharati University, Santiniketan, West Bengal India, Jan 9–13, 1998.
 17. “Assessment of genotoxicity of chemicals from structure: A computational approach” presented at the Annual Conference of the Indian Association for Cancer Congress, Calcutta, January 21–24, 1998.
 18. “Use of graph invariants in QSAR and predictive toxicology” presented at the DIMACS Workshop on Discrete Mathematical Chemistry, Rutgers University, New Jersey, March 23–25, 1998.
 19. “A computational approach to predicting toxicity: Possible applications to JP-8 jet fuel” presented at the First International Conference on the Environmental Health and Safety of Jet Fuels, San Antonio, TX, April 1–3, 1998.
 20. “Theoretical molecular descriptors for the prediction of bioactivity/toxicity, selection of analogs, discovery and optimization of leads” presented at the Astra Symposium on Advances in Medicinal Chemistry, Bangalore, India, September 17–19, 1998.
 21. “Integration of traditional Indian medicine and chemoinformatics for rapid drug discovery” presented at the conference organized jointly by East India Pharmaceutical Company, Calcutta, India, October 12, 1998.
 22. “Clustering of JP-8 constituents into structurally dissimilar groups: A novel computational strategy for predictive toxicology” presented at the Air Force Office of Scientific Research JP-8 Jet Fuel Toxicology Workshop, University of Arizona, Tucson, AZ, December 2–3, 1998.
 23. “Toxicology in silico: Addressing the quagmire of environmental pollution and protecting public health using computational chemistry” presented at the International Symposia Series: Reducing the Environmental Impacts of Toxic Chemicals in Asian Economies. The Impacts of Toxic Chemicals and Pollutants on Public Health, the Ecology and the Environment of the Bengal Basin - Bangladesh and India, Dhaka Bangladesh, on March 1, 1999.
 24. “Computational toxicology: A cost effective approach for the protection of human and environmental health” presented at the International Conference at Santiniketan, India, March 7, 1999.
 25. “The utility of Ayurvedic medicine for modern drug discovery: An exploratory analysis” presented at the conference organized by the East India Pharmaceutical Company, Calcutta, September of 1999.
 26. “Development of hierarchical QSAR models for predicting toxicity of chemicals: Statistical and neural net approaches” presented at the Air Force Predictive Toxicology Conference, Wright Patterson Air Force Base, Dayton, OH.
 27. “Exploring the scientific basis of Ayurvedic medicine: A computational approach” presented at the conference Beyond Conventional Healthcare: Understanding Alternative Choices organized by the

- University of Wisconsin, Superior, Nov., 1999.
28. "Clustering of JP-8 chemicals using structure spaces and property spaces: A computational approach" presented at the Air Force Office of Scientific Research JP-8 Jet Fuel Toxicology Workshop, University of Arizona, Tucson, Jan. 11–12, 2000.
 29. "Predicting biomedical and toxicological properties of chemicals using molecular descriptors: A hierarchical QSAR approach" presented at the International Conference on Medicinal Chemistry and Biocatalysis organized by Delhi University, India, January 26–29, 2000.
 30. "A hierarchical QSAR approach for predicting property/activity/toxicity of chemicals using theoretical structural descriptors" presented at the Second Indo-US Workshop on Mathematical Chemistry, organized by NRRI and Visva Bharati University, India; Duluth, Minnesota, May 30–June 3, 2000.
 31. "Mathematical structural invariants: Tools for drug design and predictive toxicology," presented at the international symposium on "Strategies and perspectives in drug development, design and molecular modelling," organized by the Indian Institute of Chemical Biology, Calcutta, India, October 17–18, 2000.
 32. AFOSR JP-8 jet fuel toxicology conference, January 10–12, 2001, organized at the University of Arizona, Tucson, AZ.
 33. "Use of mathematical structural invariants in computer-assisted drug design," presented at the international symposium Current Trends in Drug Design organized February 11–15, 2001, Lucknow, India.
 34. "Clustering of JP-8 chemicals using structure spaces and property spaces," presented at the Harry Wiener International Memorial Conference on the Role of Topology in Chemistry, The University of Georgia, Athens, Georgia, March 21–24, 2001.
 35. "On characterization of amino acids by the Variable Connectivity Index," presented at the Harry Wiener International Memorial Conference on the Role of Topology in Chemistry, The University of Georgia, Athens, Georgia, March 21–24, 2001.
 36. "On characterization of DNA sequences based on the occurrence of triplets of nucleic acid bases," presented at the Harry Wiener International Memorial Conference on the Role of Topology in Chemistry, The University of Georgia, Athens, Georgia, March 21–24, 2001.
 37. "On mathematical characterization of maps with applications to proteomics," presented at the Harry Wiener International Memorial Conference on the Role of Topology in Chemistry, The University of Georgia, Athens, Georgia, March 21–24, 2001.
 38. "Ordering and partial ordering of alkane isomers as a criterion for classifying topological indices" presented at the Harry Wiener International Memorial Conference on the Role of Topology in Chemistry, The University of Georgia, Athens, Georgia, March 21–24, 2001.
 39. "Applications of topological indices in predicting property/activity/ toxicity of chemicals" presented the Harry Wiener International Memorial Conference on the Role of Topology in Chemistry, The University of Georgia, Athens, Georgia, March 21–24, 2001.
 40. "Quo Vadis QSAR?," presented at the international Workshop on Molecular Structure-Property Relationships, organized at Wright State University, Dayton, OH, May 17, 2001.
 41. "Chemistry in silico as a tool for hazard assessment and drug discovery: Prospects and problems," presented at the International Congress on Computational Intelligence: Methods and Applications (CIMA 2001), organized at the University of Wales, Bangor, United Kingdom, June 19–22, 2001.
 42. "A graph theoretical approach to modeling urban development," at a conference on sustainable ecological, economic and social systems organized at the Laboratory of the Midcontinental Ecology Division, US Environmental Protection Agency, Duluth, MN, June 27–28, 2001.
 43. "Application of mathematical molecular descriptors in predicting toxicity of chemicals: A computational approach," presented at the Quantitative Structure-Toxicity Relationship symposium which was part of the Fifth Girona Seminar on Molecular Similarity, July 12–20, 2001, organized in honor of Professor Haruo Hosoya.
 44. "Applications of mathematical structural descriptors in predicting toxicity and genotoxicity of

- chemicals: A computational approach,” presented at the QSAR Workshop, August 20–22, organized at the National Center for Environmental Assessment, Cincinnati, by the United States Environmental Protection Agency.
45. “Applications of mathematical structural descriptors in hazard assessment of chemicals: Problems and prospects,” presented at the annual meeting of the Society for Risk Analysis, Seattle, Dec 2–5, 2001.
 46. “QSAR modeling of the toxicity of halogenated aliphatics,” presented at the annual meeting of the Society for Risk Analysis, Seattle, Dec 2–5, 2001.
 47. “Applications of bioinformatics and chemoinformatics in predicting bioactivity of complex mixtures,” presented at the Medicine and Veterinary Sciences section of the 89th session of the Indian National Science Congress, organized at Lucknow University, Lucknow, Uttar Pradesh, India, December, 2001.

D. Invited lectures and seminars

1. “Use of information-theoretic indices in drug design” presented at the National Cancer Institute, National Institute of Health, Bethesda, MD, July 7, 1984.
2. “The utility of graph-theoretic indices in drug design” presented at the Upjohn Company Kalamazoo, MI, January 1986.
3. “Use of topological indices in drug design and toxicological risk assessment” presented at the Monsanto company, St Louis, MO, August 1987.
4. “A graph-theoretic approach to the characterization of chemical structure” presented at the Center for Lake Superior Environmental Studies, University of Wisconsin, Superior, July 1988.
5. “Negotiating the quagmire of chemical product control: development and application of quantitative structure-activity relationships (QSAR) in predictive toxicology” presented at the Sigma Xi Lecture, University of Minnesota Duluth, December 1989.
6. “A computational approach in predicting physical and biological properties of molecules” presented at the Hormel Institute, Austin MN, July 1990.
7. “Environmental applications of QSAR” presented at the Industrial Toxicology Research Center, Lucknow, India, October 1990.
8. “Use of nonempirical parameters in QSAR studies” presented at the Central Drug Research Institute, Lucknow, India, October 1990.
9. “A rational approach to drug design and risk assessment of chemicals” delivered at the Indian Institute of Chemical Biology, Calcutta, India, October 1990.
10. “A nonempirical approach to predictive toxicology” presented at the Indian Association for the Cultivation of Science, Calcutta, India, October 1990.
11. “QSAR study: a rational approach to drug design” presented at the Department of Biochemistry, University of Calcutta, India, November 1990.
12. “A rational approach to drug design and risk assessment of environmental chemicals” presented at Organon Ltd, Calcutta, India, November 1990.
13. “A nonempirical approach to predicting Molecular properties” presented at the National Cancer Institute, Bethesda, MD, April 1991.
14. “Molecular similarity: quantification and applications” presented at the Glaxo Pharmaceutical Company at Raleigh, NC, May 1993.
15. “Development and application of molecular similarity methods for drug design and risk assessment” presented at the University of Southern California School of Pharmacy, August 3, 1993.
16. “Drug design and discovery: Molecular and computational approaches” presented at the Medical University of South Carolina, Charleston SC, December 1993.
17. “Modelling molecular properties using chemical graph theory” presented at the Oak Ridge National laboratory, TN, December 1993.
18. “The applications of chemical graph theory to predicting molecular properties” at the Center for Northern Studies of Lakehead of the Subsurface Fate and Transport Subarea Kickoff Meeting of the Air

- Force Environmental Quality Basic research program, organized by the Air Force Office of Scientific Research at the Tyndall Air Force Base, Panama City, FL, May 1994.
19. "Estimating molecular properties using chemical graph theory" presented at the Department of Chemistry and Biochemistry of Arizona State University, Tempe, March 1994.
 20. "Predicting environmental properties of chemicals using nonempirical parameters" at the University of Rome, April, 1994.
 21. "Predicting biomedical and environmental properties of chemicals using graph theoretic parameters" at the NATO Advanced Study Institute on Pharmacokinetics, Erice, Sicily, April 1994.
 22. "Applications of graph theory in chemistry, medicine, and environmental sciences" at the University of Wisconsin, Superior, April 1994, as part of the Mathematics in Medicine Week sponsored by Mathematics Association of America.
 23. "Predicting toxicity and degradability of quadricyclane, fluorocarbon ethers and their analogs," as part of the subsurface Fate and Transport Subarea Kickoff Meeting of their Force Environmental Quality Basic Research Program, organized by the Air Force Office of Scientific Research at the Tyndall air Force Base, Panama City, FL, May 1994.
 24. "Use of graph theoretic methods in risk assessment of environmental chemicals" at the National Institute of Environmental Health Sciences, Research Triangle Park, NC, July 1994.
 25. "Use of nonempirical parameters in QSAR and novel drug discovery" presented to the Pharmaceutical Discussion Group, New Delhi, India, November 1994.
 26. "Development of novel molecular similarity approaches and their applications in drug discovery" presented at the Department of Chemical Technology, University of Bombay, November 1994.
 27. "Use of graph theoretic parameters in drug design and environmental toxicology" presented at the Department of Biochemistry, University College of Science, University of Calcutta, November 1994.
 28. "A biomathematical approach to risk assessment and drug design" presented at the Bose Institute, Calcutta, December 1994.
 29. "Development of nonempirical molecular descriptors and their applications in drug design" presented at Alza Inc, Palo Alto CA, January 1995.
 30. "Use of graph theoretic approaches in the quantification of chemical similarity and structure-activity studies" presented at Stanford University, February 1995.
 31. "Use of molecular similarity methods in the risk assessment of chemicals: a study with quadricyclane" presented at the Predictive Toxicology Program review of the US Air Force Office of Scientific Research, Dayton OH May 1995.
 32. "Predicting toxicity and degradability of quadricyclane, fluorocarbon ethers and their analogs" presented at the Air Force/Army Department of Energy Joint Conference on Basic Research on Environmental Quality: Subsurface Fate and Transport, Boulder Jun, 1995.
 33. "Biological applications of chemical graph theory" at Visva Bharati University, Bolpur Santiniketan, Wet Bengal, India, March 96.
 34. "A graph theoretical approach to computational toxicology" at the Department of Biochemistry, Calcutta University, India, March 1996.
 35. "Applications of computational chemistry in biomedical research and drug discovery" at the Calcutta University Institute of Basic Medicine, India, March 1996.
 36. "Applications of computational chemistry in the risk assessment of environmental pollutants" at the All India Institute of hygiene and Public Health, Calcutta, March 1996.
 37. "Use of topological and geometrical parameters in predicting pharmacological and toxicological properties of chemicals" presented at the University of Minnesota, Pharmaceutics, Minneapolis, April 1996.
 38. "QSAR/QMSA using nonempirical parameters: applications in predictive toxicology and drug discovery" at Abbott Laboratories, Chicago, September 1996.
 39. "Development of QMSA and QSAR methods of hazard assessment of chemicals: tools for

- computational toxicology” at the Air Force Office of Research (AFOSR) Toxicology Program Review, Fairborn, OH, December 1996.
40. “Computational chemical graph theory and its practical applications” in the Scientific Computing Seminar Series, laboratory for Intelligent Systems, University of Minnesota Duluth, January 1997.
 41. “Novel Drug Design Methods: assessing activity and toxicity using computational chemistry” at the Department of Molecular Biology, and Genetics, University of Guelph, Ontario, Canada, July 3, 1998.
 42. “Use of theoretical structural descriptors in molecular design and hazard assessment of chemicals” to the scientists of the computer-aided drug design company NANODESIGN, INC, Toronto, Canada, July 6, 1998.
 43. “Prediction of bioactivity of chemicals from structure: A computational approach” at the Indian Institute of Science, Bangalore, India, September 20, 1998.
 44. “Novel drug discovery methods: Predicting pharmacological and toxicological properties of chemicals using computational chemistry” presented at the Meharry Medical College, Nashville, TN, January 19, 1999.
 45. “From graph invariants to molecular design: 25 years after the connectivity index” presented at Visva Bharati University, Santiniketan, West Bengal, India, February 11, 1999.
 46. “Theoretical molecular descriptors for the prediction of bioactivity, toxicity, selection of analogs, discovery and optimization of leads” presented at the Wockhardt Research Centre, Aurangabad, Maharashtra, India, on February 15, 1999.
 47. “Prediction of bioactivity of chemicals from structure: A hierarchical computational approach” presented at Bharatiya Vidya Bhavans Swami Prakashananda Ayurvedic Research Center, Mumbai, India, on February 18, 1999.
 48. “Novel drug discovery methods: Predicting pharmacological and toxicological properties of chemicals using computational chemistry” presented at the School of Pharmacy, Dhaka University, Dhaka, Bangladesh on March 4, 1999.
 49. “Estimation of DNA damage from toxic chemicals by graphical techniques” presented March 8, 1999.
 50. “A hierarchical QSAR approach for predicting property/activity of chemical from structure” presented at the Rugjer Boskovic Institute, Zagreb, The Republic of Croatia, September of 1999.
 51. “Predicting property/activity/toxicity of chemicals from structure: A hierarchical QSAR approach” presented at the National Institute of Chemistry, Slovenia, September of 1999.
 52. “Prediction of activity/toxicity of chemicals from structure using graph invariants” presented at the Visva Bharati University, Santiniketan, West Bengal, India, September of 1999.
 53. “Predicting biomedical and toxicological properties of chemicals using molecular descriptors” presented at the University of Delhi, India.
 54. “Applications of theoretical molecular descriptors in drug discovery and predictive toxicology: A computational approach” presented at the University of Montana, Missoula, January 6, 2000.
 55. “Applications of theoretical molecular descriptors in drug discovery and predictive toxicology: A computational approach” presented at the Ranbaxy Research Laboratories, Udyog Vihar Industrial Area, Gurgaon, Hariyana, India, January 30, 2000.
 56. “Use of mathematical descriptors in drug design and risk assessment,” presented to the biomedical scientists and practitioners of Ayurvedic medicine, February 21, 2001, Calcutta, India.
 57. Presentations and discussions on the role of QSAR in anticancer drug design with colleagues at the Josephine Ford Cancer Center, and Long Island College Hospital, New York.
 58. “Predicting therapeutic activity, health hazard and ecotoxicity of chemicals using chemodescriptors and biodescriptors: An integrated approach,” presented at the UMD Department of Biology, November 9, 2001.
 59. “Prediction of bioactivity of chemicals using chemodescriptors and biodescriptors: An integrated approach,” presented at the Ricerca, LLC Company, Concord, Ohio, November 12, 2001.
 60. “Use of Mathematical invariants in drug discovery and hazard assessment of chemicals,” presented at

- the Applied Mathematics Department, University of Calcutta, Kolkata, West Bengal, India, December, 2001.
61. “Applications of calculated molecular descriptors in drug design and risk assessment of chemicals,” presented at Shibatosh Mukherjee Science Center, Kolkata, West Bengal, India, January, 2002.
 62. “Chemistry in silico: Applications of theoretical structural invariants in drug discovery and hazard estimation of chemicals,” presented at Department of Chemistry, University of Minnesota – Duluth, February 15, 2002.
 63. “Estimation of toxicological and ecotoxicological properties of chemicals from structure: A Mathematical-cum-Computational approach,” presented to the faculty and students of the Toxicology Program of the University of Minnesota, broadcast from Duluth, MN, March 2002.
 64. “Numerical graph invariants: Development and applications in drug discovery and risk assessment of chemicals,” presented to the Department of Mathematics and Statistics, University of Minnesota Duluth, Duluth, MN, March 2002.
 65. “Interrelationship of major topological indices,” presented at the Joint Annual Meeting of the Society of Environmental Toxicology and Chemistry (Midwest Chapter) and Society of Toxicology (Northland Chapter) organized at the USEPA Mid- Continental Ecology Division, in Duluth, MN, April 2002.
 66. “Development of new tools for quantitative characterization of proteomics maps,” presented at the symposium Development and Application of Ecogenomics for Water Quality Assessment organized jointly by the Council of State Governments and the United States Environmental Protection Agency, in Kansas City, MO, May 2002.
 67. “Chemodescriptors versus biodescriptors in toxicity prediction of halocarbons,” presented at the QSAR 2002 Conference, May 25–29, 2002, Ottawa, Canada.
 68. “Predicting toxicity of chemicals in the post-genomic era: A computational approach,” delivered to the Department of Molecular Biology and Genetics, at the University of Guelph, Guelph, Ontario, Canada, June 2002.
 69. “Predicting bioactivity of chemicals from structural and proteomics-based descriptors,” presented at the University of Texas Medical Branch (UTMB) sponsored jointly by UTMB and Department of Marine Sciences, Texas A & M University at Galveston, Galveston, TX, June 2002.
 70. Dr. Basak gave the following invited seminar lectures on predictive toxicology, QSAR and Mathematical Chemistry during a trip to India in July–August 2002:
 - i. “Predicting therapeutic activity, health hazard, and ecotoxicity of chemicals using structural and proteomics based descriptors: An integrated approach,” July 26, 2002, at the Bose Institute, Kolkata, India;
 - ii. A two part lecture on “Predicting bioactivity and toxicity of chemicals from structure and proteomics based descriptors” at the Department of Biochemistry, Calcutta University, Kolkata, August 2, 2002;
 - iii. A two part lecture on “Use of discrete mathematics in chemistry, drug design and ecotoxicology,” “Part I: Molecular descriptors and QSAR,” August 7, 2002; “Part II: Molecular similarity and integrated QSAR in predictive toxicology,” August 8, 2002, at the Sivatosh Mookerjee Science Center, Kolkata, India;
 - iv. An invited lecture on “Integration of chemoinformatics and bioinformatics for drug discovery and environmental protection: An integrated approach in the post-genomic era,” at the Indian Institute of Chemical Biology, Kolkata;
 - v. “Use of mathematical invariants in drug discovery and toxicology in the post-genomic era: An *in silico* approach.”
 71. Basak presented three invited lectures at the international conference Thirty First Year of the Topological Index Z, organized by Ochanomizu University (Tokyo) and National Institute of Advanced Industrial Science and Technology (Japan), October 28–29, 2002:
 - i. “Numerical graph invariants: Development and applications in drug discovery and risk assessment of chemicals,”

- ii. "On Clustering of JP-8 Chemicals using graph invariants," and
 - iii. "Quantitative molecular similarity methods in the estimation of chemical properties and activities: A comparison of arbitrary versus tailored similarity spaces."
72. "Indigenous medicinal plants and modern drug discovery: A computational approach in the post-genomic era," presented at the meeting Science and Economy: New Insights on Medicinal Plants and Floriculture organized by Darjeeling Doohrs Postgraduates' Welfare Association (DDPGWA), Darjeeling, West Bengal, India, and Institute of Rural Development, Natural Disaster and Environmental Management, Kolkata, India, November 17, 2002.
 73. "Use of Chemo and Bio-descriptors for predicting activity/toxicity of chemicals: An Integrated QSAR approach," presented at the University Department of Chemical Technology (UDCT), University of Bombay, Mumbai, India, February 2003.
 74. "Use of chemodescriptors in drug design and hazard assessment of chemicals," presented at the Center for Bioinformatics, University of Pune, Maharashtra, India, February 2003.
 75. "Integrated modeling of bioactivity using chemo and biodescriptors," presented at the University of Pune, February 2003.
 76. "Mathematical invariants in the characterization of chemical structure, drug design, and environmental protection," presented at the Thirty Second Annual Conference of the Association for the Improvement of Mathematics Teaching (AIMT), organized at the premises of Vivekananda Math, Ramakrishna Vivekananda Mission, West Bengal, India, February 2003.
 77. "Characterization of complex Ayurvedic medicinal products: A structural-cum-mathematical approach," presented at the J. B. Ray Ayurvedic College, Kolkata, India, February 2003.
 78. "Use of mathematical structural invariants to predict properties of molecules and biomolecules," presented at the Department of Mathematics, University of Xiamen, Fujian, Peoples Republic of China, February 2003.
 79. "Use of molecular descriptors in predicting pharmacological and toxicological properties of molecules," presented to the Department of Chemistry, Xiamen University, P R China, February 2003.
 80. "Integrated QSAR for drug design and natural medicine: A computational approach," presented at Xiamen University, February 2003.
 81. "Drug design using mathematical chemical descriptors," presented at the S. N. Pradhan Center for Neurosciences, University College of Medicine, University of Calcutta, Kolkata, India, February 2003.
 82. "Chemodescriptors and biodescriptors: Development and applications in drug discovery and hazard assessment of chemicals," presented at the National Institute of Chemistry, Ljubljana, Slovenia, March 2003.
 83. "Applications of chemodescriptors and biodescriptors in predicting therapeutic and toxic properties of chemicals," presented at the Rugjer Boskovic Institute, The Republic of Croatia, March 2003.
 84. "Estimation of blood: Air partition coefficients of volatile organic chemicals using molecular descriptors," presented at the 2003 Toxicology and Risk Assessment Conference, April 28–May 1, in Fairborn, Ohio.
 85. "Use of calculated structural descriptors in predicting toxicity of chemicals," presented at the Conference on the Prediction of Acute Toxicity, May 1–2, 2003, organized by the MITRE Corporation, Washington, DC.
 86. "Chemodescriptors and biodescriptors: Development and applications in drug design and hazard assessment of chemicals," presented at Stanford University, Palo Alto, CA, May 2003.
 87. "Predicting membrane permeability using HiQSAR," presented at the JP8 Toxicology Conference, May 14–16, 2003, organized at the University of Arizona Medical Center, Tucson, AZ.
 88. "The role of chemodescriptors and biodescriptors in drug design and predictive toxicology," presented at the Chemoinformatics Symposium at the Intelligent Drug Discovery and Development Conference, May 28-30, 2003, organized by the Cambridge Health Institute, Philadelphia, Penn.
 89. "Use of chemodescriptors and proteomics-based biodescriptors in predictive toxicology: A computational approach," a two-part lecture presented at the ImageTox conference of the European

- Community organized at the University of Tartu, Estonia, June 2003.
90. "Mathematical descriptors in predicting activity/toxicity of chemicals," presented at the Department of Crystallography, Birkbeck College, University of London, June 2003.
 91. "Predicting toxicity of chemicals using chemodescriptors and biodescriptors," presented at the Sixth Girona Seminar on Molecular Similarity, July 21–24, 2003, organized at the University of Girona, Spain.
 92. "Applications of chemodescriptors and biodescriptors in predictive toxicology: An integrated approach," presented at the Third Indo-US Workshop for Mathematical Chemistry, August 2–7, 2003, University of Minnesota Duluth.
 93. "Use of mathematical biodescriptors and chemodescriptors in predicting toxicity of chemicals," presented at the International Symposium on Water: Crisis and Strategies, organized jointly by the International Institute of Bengal Basin and Center for Ground Water Studies in Kolkata, India, February 7–8, 2004.
 94. Dr. Basak made the following presentations at the Current Trends in Drug Discovery Research (CTDDR) conference in Lucknow, India, February 17–20, 2004:
 - i. "Prediction of bioactivity/ toxicity of chemicals using proteomics based mathematical descriptors," and
 - ii. "Applications of theoretical molecular descriptors in QSAR modeling of anti-mycobacterial compounds."
 95. "Prediction of toxicity of chemicals using chemodescriptors and biodescriptors," presented at the 11th International Workshop on Quantitative Structure-Activity Relationships in the Human Health and Environmental Sciences, Liverpool, England, June 2004.
 96. "Use of mathematical biodescriptors and chemodescriptors in predicting bioactivity/toxicity of chemicals," presented at the Memorial Symposium on Molecular Informatics, Modeling and Simulation, on June 23–26, 2004 at Memorial University of Newfoundland, St John's, Newfoundland, Canada.
 97. "Mathematical chemodescriptors and biodescriptors in biological structure-activity relationships," presented at the Southwest Theoretical Chemistry Conference XXI, Galveston, TX, October 22–23, 2004.
 98. "Mathematical structural invariants: Developments and applications," presented at the Fourth Indo-US Workshop for Mathematical Chemistry, organized in Pune, Maharashtra, India, January 8–12, 2005.
 99. "Advancing frontiers of graph-theoretic applications in environmental protection and drug design," presented at the conference Graph Theory and its Applications in Pollution Prevention and Drug Design: An International Conference Honoring Frank Harary, held on January 18, 2005 in Kolkata, India.
 100. "Computer-assisted estimation of blood:air partition coefficients of VOCs: Implications for chemical mixtures," presented at the international conference Contemporary Concepts in Toxicology-Charting the Future: Building the Scientific Foundation for Mixtures Joint Toxicity and Risk Assessment, organized by the Agency for Toxic Substance and Disease Registry (ATSDR), Centers for Disease Control and Prevention, Atlanta, GA, February 16–17, 2005.
 101. "Predicting bioactivity and toxicity of chemicals from computational chemistry and mathematical proteomics," presented at the Conferentia Chemometrica 2005 in Hajdúszoboszló, Hungary, August 28–30.
 102. "A comparative study of arbitrary versus tailored molecular similarity metrics in property/toxicity/ bioactivity prediction," presented at the International Conference of Computational Methods in Sciences and Engineering 2005 in Korinthos, Greece, October 21–26.
 103. "Use of proteomics-based biodescriptors versus chemodescriptors in predicting halocarbon toxicity: An integrated approach," presented at the International Conference of Computational Methods in Sciences and Engineering 2005 in Korinthos, Greece, October 21–26.
 104. "The role of chemodescriptors and biodescriptors in predicting bioactivity and toxicity," presented at

- the Computational Methods in Toxicology and Pharmacology conference, Shanghai, PRC, October 29 – November 1, 2005.
105. “Combining modern drug discovery methods with biodiversity of Darjeeling plants in the discovery of pharmaceuticals and cosmeceuticals,” presented at an international conference on Drug Discovery Based on Darjeeling Area Biodiversity, held November 7, 2005.
 106. “Advancing frontiers of mathematical chemistry,” presented in a mini-symposium at a conference on Current Advances in QSAR Studies in Kolkata, India, held November 8, 2005.
 107. “The utility of mathematical descriptors in the prediction of property, biochemical activity and toxicity of chemicals,” presented at the Department of Biochemistry, University of Calcutta, Kolkata, India, November 21, 2005.
 108. “Theoretical descriptor-based QSARs in predicting skin penetration of chemicals,” presented at the AFOSR JP-8 Jet Fuel Toxicology Meeting, University of Arizona, Tucson, November 30–December 2, 2005.
 109. “Clustering and QSAR of JP8 fuel chemicals,” presented at the Jet Fuel Meeting “Integrating models on lung disposition and toxicokinetics of jet fuels” organized at the Mechanical and Aerospace Engineering Department of NCSU, January 2006.
 110. “Prediction of halocarbon toxicity using chemodescriptors and proteomics based biodescriptors: An integrated approach,” presented at the 12th International Workshop on Quantitative Structure-Activity Relationships in Environmental Chemistry (QSAR 2006), May 8–12, in Lyon, France.
 111. “Mathematical descriptors in the classification/ prediction of biological processes,” presented in Dubrovnik, Croatia at the meeting of the International Academy of Mathematical Chemistry (IAMC), June 15–17, 2006.
 112. “Prediction of tissue partition co-efficients using mathematical structural descriptors versus experimental properties,” presented at the 21st Dubrovnik International Course and Conference on the interfaces among Mathematics, Chemistry and Computer Sciences (Math/Chem/Comp 2006), Dubrovnik, Croatia, June 19–24, 2006.
 113. “Applications of mathematical chemistry in modern drug discovery and environmental protection,” presented at the Ramakrishna Mission Vivekananda University, November 2, 2006.
 114. “Advancing frontiers of mathematical chemistry,” presented at the First Indo-U.S. Lecture Series on Discrete Mathematical Chemistry on January 8–11, 2007, PES Institute of Technology, Bangalore, India.
 115. “Predicting skin penetration and interaction with JP-8,” presented at the JP-8 jet fuel conference organized by the U.S. Air Force, Tucson, AZ, January 17–19, 2007.
 116. “Chemo-bioinformatics: Characterization of molecules and biomolecules using mathematical descriptors,” keynote lecture given at the 15th International Symposium on Spectroscopy in Theory and Practice, April 18–21, 2007, Nova Gorica, Slovenia.
 117. “DNA and proteomics-based biodescriptors and their applications,” presented at the National Institute of Chemistry, Ljubljana, Slovenia, April 23, 2007.
 118. “Development and applications of chemodescriptors,” presented at the National Institute of Chemistry, Ljubljana, Slovenia, April 24, 2007.
 119. “Mathematical descriptors of proteomics maps and their biological applications,” presented in Dubrovnik, Croatia, June 7, 2007.
 120. “Chemodescriptors and biodescriptors: Mathematical basis and applications,” a specialized two-lecture course presented at the 22nd International Course & Conference on the Interfaces among Mathematics, Chemistry & Computer Sciences, Dubrovnik, Croatia, June 11–16, 2007.
 121. “Use of arbitrary and tailored molecular similarity methods in the estimation of property/ bioactivity of chemicals,” presented at the 22nd International Course & Conference on the Interfaces among Mathematics, Chemistry & Computer Sciences, Dubrovnik, Croatia, June 11–16, 2007.
 122. “Background and History of the Mathematical Chemistry Lecture Series,” presented at the Second Indo-US Lecture Series on Discrete Mathematical Chemistry, Kalpetta, Kerala, India, June 2007.

123. "Mathematical Structure Descriptors: Development and applications in chemistry, drug discovery, environmental protection, and bioinformatics," presented at the Second Indo-US Lecture Series on Discrete Mathematical Chemistry, Kalpetta, Kerala, India, June 2007.
124. "Realizing a balance via Mathematical Chemistry," presented at the Second Indo-US Lecture Series on Discrete Mathematical Chemistry, Kalpetta, Kerala, India, June 2007.
125. The first A. N. Bhaduri Memorial Lecture, "Modeling in drug design and environmental protection," presented at the B. C. Guha Center for Genetic Engineering and Biotechnology, University of Calcutta, organized jointly by Science for Society (India) in collaboration with the Eastern India Chapter of the International Society of Mathematical Chemistry on July 3, 2007, Kolkata, West Bengal, India.
126. "Estimation of tissue partitioning of chemicals from their structure: A hierarchical QSAR approach," presented at the Computational Chemistry Maui Workshop 2007 organized by the Defense Threat Reduction Agency, Chemical and Biological Technologies and Threat Agency Sciences, US Department of Defense, 13–16 August, 2007.
127. "Mathematical biodescriptors of proteomics maps and their toxicological applications," presented at the Computational Chemistry Maui Workshop 2007 organized by the Defense Threat Reduction Agency, Chemical and Biological Technologies and Threat Agency Sciences, US Department of Defense, 13–16 August, 2007.
128. "Predicting allergic contact dermatitis: alternative statistical approaches to chemical classification," presented at the 234th ACS National Meeting, August 19–23, 2007.