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Present Position

Computational Chemistry Research Coordinator
Center for Water and the Environment
Natural Resources Research Institute
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Research Areas

Mathematical chemistry	Structure-activity relationship (SAR) modeling
Predictive toxicology	Environmental chemistry
Statistical model validation	Drug design

Education

BS Chemistry/Biology, *cum laude*, University of Minnesota Duluth, 1992

Honors and Awards

2004 Statistics in Chemistry Award – American Statistical Association
1992 Outstanding Graduating Chemistry Major Award—American Chemical Society
Phi Kappa Phi Honor Society

Professional Affiliations

American Chemical Society
QSAR and Modelling Society

Publications (Peer-reviewed journal articles and book chapters)

- [1] A.T. Balaban, D. Mills, and S.C. Basak, *Correlation between structure and normal boiling points of acyclic carbonyl compounds*, J. Chem. Inf. Comput. Sci. 39 (1999), pp. 758-764.

- [2] A.T. Balaban, S.C. Basak, and D. Mills, *Normal boiling points of 1, ω -Alkanedinitriles: The highest increment in a homologous series*, J. Chem. Inf. Comput. Sci. 39 (1999), pp. 769-774.
- [3] A.T. Balaban, D. Mills, O. Ivanciuc, and S.C. Basak, *Reverse Wiener indices*, Croat. Chem. Acta 73 (2000), pp. 923-941.
- [4] M. Randic, D. Mills, and S.C. Basak, *On characterization of physical properties of amino acids*, Int. J. Quant. Chem. 80 (2000), pp. 1199-1209.
- [5] S.C. Basak and D. Mills, *Prediction of mutagenicity utilizing a hierarchical QSAR approach*, SAR QSAR Environ. Res. 12 (2001), pp. 481-496.
- [6] S.C. Basak and D. Mills, *Use of mathematical structural invariants in the development of QSPR models*, MATCH (Commun. Math. Comput. Chem.) 44 (2001), pp. 15-30.
- [7] S.C. Basak, D.R. Mills, A.T. Balaban, and B.D. Gute, *Prediction of mutagenicity of aromatic and heteroaromatic amines from structure: A hierarchical QSAR approach*, J. Chem. Inf. Comput. Sci. 41 (2001), pp. 671-678.
- [8] S.C. Basak and D. Mills, *Quantitative structure-property relationships (QSPRs) for the estimation of vapor pressure: A hierarchical approach using mathematical structural descriptors*, J. Chem. Inf. Comput. Sci. 41 (2001), pp. 692-701.
- [9] B.D. Gute, G.D. Grunwald, D. Mills, and S.C. Basak, *Molecular similarity based estimation of properties: A comparison of structure spaces and property spaces*, SAR QSAR Environ. Res. 11 (2001), pp. 363-382.
- [10] A.T. Balaban, D. Mills, and S.C. Basak, *Alkane ordering as a criterion for similarity between topological indices: Index J as a "sharpened Wiener index"*, MATCH (Commun. Math. Comput. Chem.) 45 (2002), pp. 5-26.
- [11] S.C. Basak, D. Mills, D.M. Hawkins, and H.A. El-Masri, *Prediction of tissue:air partition coefficients: A comparison of structure-based and property-based methods*, SAR QSAR Environ. Res. 13 (2002), pp. 649-665.
- [12] S.C. Basak, B.D. Gute, and D. Mills, *Quantitative molecular similarity analysis (QMSA) methods for property estimation: A comparison of property-based, arbitrary, and tailored similarity spaces*, SAR QSAR Environ. Res. 13 (2002), pp. 727-742.
- [13] S.C. Basak, D. Mills, B.D. Gute, G.D. Grunwald, and A.T. Balaban, *Applications of topological indices in property/bioactivity/toxicity prediction of chemicals*, in *Topology in Chemistry: Discrete Mathematics of Molecules*, D.H. Rouvray and R.B. King, eds., Horwood Publishing Limited, Chichester, England, 2002, pp. 113-184.
- [14] S.C. Basak, B.D. Gute, D. Mills, K. Balasubramanian, K. Geiss, M. Randic, F. Witzmann, and M. Vracko, *Chemodescriptors versus biodescriptors in toxicity*

prediction of halocarbons, presented at the QSAR 2002 Conference, May 25-29, 2002, in Ottawa, Canada, (2002),

- [15] B.D. Gute, S.C. Basak, D. Mills, and D.M. Hawkins, *Tailored similarity spaces for the prediction of physicochemical properties*, Internet Electronic J. Mol. Design 1 (2002), pp. 374-387.
- [16] R. Natarajan, I. Nirdosh, S.C. Basak, and D. Mills, *QSAR modeling of flotation collectors using principal components extracted from topological indices*, J. Chem. Inf. Comput. Sci. 42 (2002), pp. 1425-1430.
- [17] S.C. Basak, K. Balasubramanian, B.D. Gute, D. Mills, A. Gorczynska, and S. Roszak, *Prediction of cellular toxicity of halocarbons from computed chemodescriptors: A hierarchical QSAR approach*, J. Chem. Inf. Comput. Sci. 43 (2003), pp. 1103-1109.
- [18] S.C. Basak, B.D. Gute, D. Mills, and D.M. Hawkins, *Quantitative molecular similarity methods in the property/toxicity estimation of chemicals: A comparison of arbitrary versus tailored similarity spaces*, J. Mol. Struct. (Theochem) 622 (2003), pp. 127-145.
- [19] S.C. Basak, D. Mills, D.M. Hawkins, and H. El-Masri, *Prediction of human blood:air partition coefficient: A comparison of structure-based and property-based methods*, Risk Analysis 23 (2003), pp. 1173-1184.
- [20] S.C. Basak and D. Mills, *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)*, in *Oxygen- and Sulfur-Containing Heterocycles, Vol. 1*, V.G. Karstev, ed., IBS Press, Moscow, 2003, p. 168.
- [21] S.C. Basak, D. Mills, M.M. Mumtaz, and K. Balasubramanian, *Use of topological indices in predicting aryl hydrocarbon receptor binding potency of dibenzofurans: A hierarchical QSAR approach*, Indian J. Chem. 42A (2003), pp. 1385-1391.
- [22] S.C. Basak, D. Mills, B.D. Gute, and D.M. Hawkins, *Predicting mutagenicity of congeneric and diverse sets of chemicals using computed molecular descriptors: A hierarchical approach*, in *Quantitative Structure-Activity Relationship (QSAR) Models of Mutagens and Carcinogens*, R. Benigni, ed., CRC Press, Boca Raton, FL, 2003, pp. 207-234.
- [23] D.M. Hawkins, S.C. Basak, and D. Mills, *Assessing model fit by cross-validation*, J. Chem. Inf. Comput. Sci. 43 (2003), pp. 579-586.
- [24] M.C. Bagchi, B.C. Maiti, D. Mills, and S.C. Basak, *Usefulness of graphical invariants in quantitative structure-activity correlations of tuberculostatic drugs of isonicotinic acid hydrazide type*, J. Mol. Modeling 10 (2004), pp. 102-111.

- [25] A.T. Balaban, S.C. Basak, A. Beteringhe, D. Mills, and C.T. Supuran, *QSAR study using topological indices for inhibition of carbonic anhydrase II by sulfanilamides and Schiff bases*, Mol. Diversity 8 (2004), pp. 401-412.
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- [27] D.M. Hawkins, S.C. Basak, and D. Mills, *QSARs for chemical mutagens from structure: ridge regression fitting and diagnostics*, Environ. Toxicol. Pharmacol. 16 (2004), pp. 37-44.
- [28] M. Randic, M. Pompe, D. Mills, and S.C. Basak, *Variable connectivity index as a tool for modeling structure-property relationships*, Molecules 9 (2004), pp. 1177-1193.
- [29] M. Vracko, D. Mills, and S.C. Basak, *Structure-mutagenicity modeling using counter propagation neural networks*, Environ. Toxicol. Pharmacol. 16 (2004), pp. 25-36.
- [30] S.C. Basak, R. Natarajan, and D. Mills, *Structure-activity relationships for mosquito repellent aminoamides using the hierarchical QSAR method based on calculated molecular descriptors*, in *Conference Proceedings: WSEAS Transactions on Information Science and Applications*, 2005, pp. 958-963.
- [31] S.C. Basak, R. Natarajan, D. Mills, D.M. Hawkins, and J.J. Kraker, *Quantitative structure-activity modeling of insect juvenile hormone activity of 2,4-dienoates using computed molecular descriptors*, SAR QSAR Environ. Res. 16 (2005), pp. 581-606.
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- [34] S.C. Basak and D. Mills, *Development of quantitative structure-activity relationship models for vapor pressure estimation using computed molecular descriptors*, ARKIVOC 2005 (2005), pp. 308-320.
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- [36] S.C. Basak, D. Mills, B.D. Gute, and R. Natarajan, *Predicting pharmacological and toxicological activity of heterocyclic compounds using QSAR and molecular modeling*, 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, 2006, pp. 39-80.

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- [40] S.C. Basak, B.D. Gute, and D. Mills, *Similarity methods in analog selection, property estimation and clustering of diverse chemicals*, *ARKIVOC* 2006 (2006), pp. 157-210.
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- [43] S.C. Basak, D. Mills, D.M. Hawkins, and J.J. Kraker, *Proper statistical modeling and validation in QSAR: A case study in the prediction of rat fat:air partitioning*, in *Computation in Modern Science and Engineering, Proceedings of the International Conference on Computational Methods in Science and Engineering 2007 (ICCMSE 2007)*, T.E. Simos and G. Maroulis, eds., American Institute of Physics, Melville, New York, 2007, pp. 548-551.
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- [45] J.J. Kraker, D.M. Hawkins, S.C. Basak, R. Natarajan, and D. Mills, *Quantitative structure-activity relationship (QSAR) modeling of juvenile hormone activity: Comparison of validation procedures*, *Chemometr. Intell. Lab. Syst.* 87 (2007), pp. 33-42.
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- [49] S.C. Basak, D. Mills, R. Natarajan, and B.D. Gute, *Predicting chemical reactivity and bioactivity from structure: A mathematical-cum-computational approach*, in *Theory of Chemical Reactivity*, P.K. Chattaraj, ed., Taylor & Francis, in press
- [50] S.C. Basak and D. Mills, *Predicting vapor pressure of chemicals from structure: A comparison of graph theoretic versus quantum chemical descriptors*, SAR QSAR Environ. Res., in press.
- [51] S.C. Basak and D. Mills, *Mathematical chemistry and chemobioinformatics: A holistic view involving optimism, intractability, and pragmatism*, in *Proceedings of the 22nd International Course & Conference on the Interfaces Among Mathematics, Chemistry & Computer Sciences; Math/Chem/Comp 2007*, A. Graovac and I. Gutman, eds., in press.
- [52] S.C. Basak, D. Mills, and B.D. Gute, *Predicting Bioactivity and Toxicity of Chemicals from Mathematical Descriptors: A Chemical-cum-Biochemical Approach*, in *Advances in Quantum Chemistry*, D.J. Klein and E. Brandas, eds., Elsevier, in press.
- [53] S.C. Basak, D. Mills, D.M. Hawkins, and J.J. Kraker, *Quantitative Structure-Activity Relationship (QSAR) Modeling of Human Blood: air Partitioning with Proper Statistical Methods and Validation*, Chemistry & Biodiversity, accepted.
- [54] S.C. Basak, D. Mills, R. Garg, and B. Bhatarai, *A QSAR study of HIV protease inhibitors using theoretical descriptors*, Curr. Comp. Aided Drug Des., submitted.
- [55] S.C. Basak, D. Mills, B.D. Gute, A.T. Balaban, K. Basak, and G.D. Grunwald, *Use of mathematical structural invariants in analyzing combinatorial libraries: A case study with Psoralen derivatives*, in *Some Aspects of Mathematical Chemistry*, D.K. Sinha, S.C. Basak, R.K. Mohanty, and I.N. Basumallick, eds., Visva-Bharati University, India, submitted.

Presentation of Research Results at Scientific Conferences

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, St. Augustine, FL: "On use of the variable connectivity index for characterization of amino acids," D. Mills, M. Randic, and S. C. Basak.

The Second Indo-US Workshop on Mathematical Chemistry, with Applications to Drug Discovery, Environmental Toxicology, Cheminformatics and Bioinformatics, May 30 – June 3, 2000, University of Minnesota, Duluth, USA: “Clustering of JP-8 chemicals using property spaces and structure spaces: A novel tool for hazard assessment.”

The 220th American Chemical Society National Meeting, Washington, DC, August 20-24, 2000:

1. “Use of variable connectivity indices on biological molecules,” D. Mills, M. Randic, and S. C. Basak.
2. “Hierarchical clustering of Psoralen derivatives using topological invariants: A strategy for molecular design,” D. Mills, S. C. Basak, B. D. Gute, A. T. Balaban, G. D. Grunwald, and K. Basak.
3. “Clustering of JP-8 chemicals using structure spaces and property spaces: A computational approach,” D. Mills, S. C. Basak, G. D. Grunwald, B. D. Gute, and J. Riviere.

International Chemical Congress of Pacific Basin Societies (Pacifichem 2000), December 14-19, 2000, Honolulu, Hawaii:

1. “Use of variable molecular descriptors for the characterization of biological molecules,” D. Mills, M. Randic, S. C. Basak.
2. “Hierarchical use of structural invariants in the clustering of a virtual Psoralen combinatorial library,” D. Mills, S. C. Basak, B. Gute, G. Grunwald, A. T. Balaban, K. Basak.

Eighteenth Annual Sigma Xi Scientific Poster Exhibition, February 18, 2002, Duluth, Minnesota, UMD School of Medicine:

1. “Prediction of Blood:Air Partition Coefficients of Volatile Organic Chemicals Using Theoretical Descriptors,” Denise Mills, Subhash C. Basak, Hisham El-Masri, and Douglas M. Hawkins.
2. “Quantitative Molecular Similarity Methods in the Estimation of Chemical Properties and Activities: A Comparison of Arbitrary Versus Tailored Similarity Spaces,” Denise Mills, Subhash C. Basak, Brian D. Gute, and Douglas M. Hawkins

Joint meeting of the Midwest Regional Chapter of SETAC (Society of Environmental Toxicology and Chemistry) & the Northland Chapter of SOT (Society of Toxicology), U. S. Environmental Protection Agency, Duluth, Minnesota, April 9-10, 2002.

1. “Hierarchical quantitative structure-toxicity relationship (Hi-QSTR) modeling of chemical toxicity,” Denise Mills, Subhash C. Basak and Brian D. Gute.
2. “Prediction of blood:air partition coefficients of volatile organic chemicals using theoretical molecular descriptors,” Denise Mills, Subhash C. Basak, Hisham El-Masri, Douglas M. Hawkins, and Brian D. Gute.

The International Conference on Chemical Mixtures (ICCM 2002), sponsored by the Agency for Toxic Substances and Disease Registry of the Centers for Disease Control, Atlanta, GA, September 10-12, 2002.

1. “Mutagen/ Non-mutagen Classification of Congeneric and Diverse Sets of Chemicals Using Computed Molecular Descriptors: A Hierarchical Approach,” Denise Mills, Subhash C. Basak, Douglas M. Hawkins and Brian D. Gute.
2. “Hierarchical Quantitative Structure-Toxicity Relationship (Hi-QSTR) Modeling of Chemical Toxicity,” Denise Mills, Subhash C. Basak, and Brian D. Gute.
3. “Estimation of Blood:Air Partition Coefficients of Volatile Organic Chemicals Using Molecular Descriptors,” Denise Mills, Subhash C. Basak, Hisham El-Masri, Douglas M. Hawkins, and Brian D. Gute.

The 2003 Toxicology and Risk Assessment Conference, Fairborn, OH, April 28, 2003 – May 1, 2003.

1. “Estimation of Blood:Air Partition Coefficients of Volatile Organic Chemicals Using Molecular Descriptors, Denise Mills, Subhash C. Basak, Hisham El-Masri, Moiz M. Mumtaz, Douglas M. and, Brian D. Gute.
2. “Hierarchical Quantitative Structure-Toxicity Relationship (Hi-QSTR) Modeling of Chemical Toxicity, Denise Mills, Subhash C. Basak, and Brian D. Gute.

The Third Indo-US Workshop on Mathematical Chemistry, with Applications to Drug Discovery, Environmental Toxicology, Cheminformatics and Bioinformatics, Duluth, MN August 2-7, 2003:

1. “Estimation of Blood:Air Partition Coefficients of Volatile Organic Chemicals Using Molecular Descriptors,” Denise Mills, Subhash C. Basak, Brian D. Gute, Hisham El-Masri, Moiz M. Mumtaz, Douglas M. Hawkins.
2. “Estimation of Estrogen Receptor Binding Affinity Using Theoretical Molecular Descriptors,” Denise Mills, Subhash C. Basak, and Douglas M. Hawkins.
3. “Hierarchical Quantitative Structure-Toxicity Relationship (Hi-QSTR) Modeling Of Chemical Toxicity,” Denise Mills, Subhash C. Basak, and Brian D. Gute.
4. “Use of Calculated Molecular Descriptors in Quantitative Structure-Activity Relationship Modelling of 2-Substituted Isonicotinic Acid Hydrazide,” Denise Mills, M.C. Bagchi, B.C. Maiti, and Subhash C. Basak.
5. “Use of Topological Indices in Predicting Aryl Hydrocarbon (Ah) Receptor Binding Affinity of Dibenzofurans: A Hierarchical QSAR Approach,” Denise Mills, Subhash C. Basak, Moiz M. Mumtaz, and Krishnan Balasubramanian.
6. “Estimation of Tissue:Air Partition Coefficients: A Comparison Of Structure- And Property-Based Methods,” Denise Mills, Subhash C. Basak, Douglas M. Hawkins, and Hisham El-Masri.

The 11th International Workshop on Quantitative Structure-Activity Relationships in the Human Health and Environmental Sciences (QSAR 2004), Liverpool, England, May 9 – 13, 2004:

1. “Estimation of blood:air partition coefficients of volatile organic chemicals using molecular descriptors,” Denise Mills, Subhash C. Basak, Brian D. Gute, Hisham El-Masri, Moiz M. Mumtaz, and Douglas M. Hawkins.
2. “Estimation of Estrogen Receptor Binding Affinity Using Theoretical Molecular Descriptors,” Denise Mills, Subhash C. Basak, and Douglas M. Hawkins.
3. “Use of Topological Indices in Predicting Aryl Hydrocarbon (Ah) Receptor Binding Affinity of Dibenzofurans: A Hierarchical QSAR Approach,” Denise Mills, Subhash C. Basak, Moiz M. Mumtaz, and Krishnan Balasubramanian.
4. “Estimation of tissue:air partition coefficients: a comparison of structure- and property-based methods,” Denise Mills, Subhash C. Basak, Douglas M. Hawkins, and Hisham El-Masri.

Computational Chemical Dynamics Symposium, University of Minnesota, Minneapolis, October 7-9, 2004.

1. “Hierarchical Quantitative Structure-Activity Relationship (HiQSAR) studies of mosquito repellency of alicyclic carboxamides,” Denise Mills, Subhash C. Basak, and Ramanathan Natarajan.
2. “Use of topological indices in predicting aryl hydrocarbon (Ah) receptor binding affinity of dibenzofurans: A hierarchical QSAR approach,” Denise Mills, Subhash C. Basak, Moiz M. Mumtaz, and Krishnan Balasubramanian.
3. “Estimation of tissue:air partition coefficients: a comparison of structure- and property-based methods,” Denise Mills, Subhash C. Basak, Douglas M. Hawkins, and Hisham El-Masri.

4. "Use of Calculated Chemodescriptors in Toxicity Prediction of Halocarbons, Denise Mills, Brian D. Gute, Subhash C. Basak, and Krishnan Balasubramanian.

The XXI Southwest Theoretical Chemistry Conference, Texas A&M University, Galveston, Texas, October 22-24, 2004.

1. "Predicting antimycobacterial activity of quinolone derivatives using theoretical molecular descriptors," Denise Mills, Manish C. Bagchi, Bhim C. Maiti, and Subhash C. Basak.
2. "Estimation of tissue:air partition coefficients: a comparison of structure- and property-based methods," Denise Mills, Subhash C. Basak, Douglas M. Hawkins, and Hisham El-Masri.
3. "Estimation of blood:air partition coefficients of volatile organic chemicals using molecular descriptors," Denise Mills, Subhash C. Basak, Brian D. Gute, Hisham El-Masri, Moiz M. Mumtaz, and Douglas M. Hawkins.
4. "Estimation of estrogen receptor binding affinity using theoretical molecular descriptors," Denise Mills, Subhash C. Basak, Denise Mills, and Douglas M. Hawkins.
5. "Use of topological indices in predicting aryl hydrocarbon (Ah) receptor binding affinity of dibenzofurans: A hierarchical QSAR approach," Denise Mills, Subhash C. Basak, Moiz M. Mumtaz, and Krishnan Balasubramanian.
6. "Use of calculated chemodescriptors in toxicity prediction of halocarbons," Denise Mills, Brian D. Gute, Subhash C. Basak, and Krishnan Balasubramanian.

Cambridge Healthtech Institute's 2nd Annual Predictive ADME and Predictive Toxicology Conference, San Diego, CA, January 11-12, 2005.

1. "Predicting blood:air partition coefficients using calculated molecular descriptors," Denise Mills, Subhash C. Basak, Brian D. Gute, Hisham A. El-Masri, Moiz M. Mumtaz, and Douglas M. Hawkins.
2. "Predicting estrogen receptor binding affinity using theoretical molecular descriptors," Denise Mills, Subhash C. Basak, and Douglas M. Hawkins.