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EDUCATION:

1982-1986 Ph.D., Biochemistry and Pharmacology, Moscow State University, Moscow, USSR. Advisor: Prof Lev S. Yaguzhinski. Thesis: Quantitative Structure-Activity Relationships for Muscarinic and Nicotinic Agonists and Antagonists.

1977-1982 M.S., Chemistry, Moscow State University, Moscow, USSR.

PROFESSIONAL EXPERIENCE:

2015-2016 K.H. Lee Distinguished Professor and Associate Dean for Pharmacoinformatics and Data Science, UNC Eshelman School of Pharmacy, UNC- Chapel Hill

2011-2015 K.H. Lee Distinguished Professor and Associate Dean for Research and Graduate Education, UNC Eshelman School of Pharmacy, UNC- Chapel Hill

2005-2011 K.H. Lee Distinguished Professor and Chair, Division of Medicinal Chemistry and Natural Products, UNC Eshelman School of Pharmacy, UNC- Chapel Hill

2004 –present Full Professor, Division of Medicinal Chemistry and Natural Products, UNC Eshelman School of Pharmacy, UNC- Chapel Hill

1997-2004 Associate Professor, Division of Medicinal Chemistry and Natural Products, School of Pharmacy, UNC- Chapel Hill

1991-present Director, Laboratory for Molecular Modeling, Division of Medicinal Chemistry and Natural Products, School of Pharmacy, UNC- Chapel Hill (primary appointment).

1991-1997 Assistant Professor, Division of Medicinal Chemistry and Natural Products, School of Pharmacy, UNC- Chapel Hill

2001-present Adjunct Associate (until 2004), Adjunct Full Professor, Department of Biomedical Engineering, School of Medicine, The University of North Carolina at Chapel Hill.

2008-present Adjunct Professor**,** Department of Computer Science, UNC-Chapel Hill.

2001-2006 Associate Director, Carolina Center for Genome Sciences, UNC-Chapel Hill.

2002-2006 Founding Director, UNC Graduate Training Program in Bioinformatics and Computational Biology.

2001-2004 Director, Duke-UNC Training Program in Medical Informatics.

2000-2002 Director of Graduate Studies, MCNP Division, School of Pharmacy

1989-1991 UNC Postdoctoral Fellow/Trainee (with J.S.Kizer, M.D. J.P.Bowen, Ph.D. and J. Hermans, Ph.D.), Brain and Development Research Center, UNC-Chapel Hill.

1988-1988 Research Scientist, Research Institute of Biotechnology, Moscow, USSR

1986-1988 Postdoctoral Fellow (with Prof. L.S.Yaguzhinsky), Moscow State University, Moscow, USSR, Laboratory of Molecular Biology and Bioorganic Chemistry.

HONORS:

-Graduated *summa cum laude*, Moscow State University, 1982.
-Recipient of 1992 Tripos Inc. Academic User of the Year Award.

-Recipient of 1993 Chairman's Award, North Carolina Section of the American Chemical Society.
-Vice-Chair, Cheminformatics and QSAR Society, 2005-present.
-External Fellow, Center for the Study of Biological Complexity, VCU, 2004-present
-Visiting Professor, Louis Pasteur University of Strasbourg, France, 2006
-K.H. Lee Distinguished Professor, School of Pharmacy, 2008.
- Lena Joels Research Foundation Visiting Professor, Faculty of Medicine, Hebrew University of Jerusalem, Jerusalem, Israel, 2011
-Academic Research Fellow, AACP, 2013-2014
-Co-Chair, International Advisory Board, Skoltech University, Moscow, Russia, 2014-
-Associate Editor, Journal of Chemical Information and Modeling, American Chemical Society, 2015-

RESEARCH INTERESTS:

Computational Chemistry, Cheminformatics, Structural Bioinformatics, Computational Toxicology, Materials Informatics.

BIBLIOGRAPHY (asterisk indicates the senior author)

(h-index=57 per GoogleScholar: https://scholar.google.com/citations?user=inPIy48AAAAJ&hl=en).

Books and Chapters:

1. Fourches, D.; **Tropsha, A**.* Quantitative Nanostructure-Activity Relationships: from Unstructured Data to Predictive Models for Designing Nanomaterials with Controlled Properties. In *Nanotoxicology: Progress toward Nanomedicine*; Monteiro-Riviere, N. A.; Lang Tran, C., Eds.; CRC Press, **2014** (03/2014; ISBN: 9781482203875)
2. Golbraikh, A., Wang, X.S., Zhu, H., and **Tropsha, A***. Predictive QSAR Modeling: Methods and Applications in Drug Discovery and Chemical Risk Assessment. In: Handbook of Computational Chemistry, Shukla and Leshinkii, Eds, Springer, **2012**, pp. 1309-1342.
3. **Tropsha, A**. Recent Advances in Development, Validation, and Exploitation of QSAR Models. In: *Burger's Medicinal Chemistry and Drug Discovery*, Abraham, D., Ed., Seventh Edition. Volume 1. New York: John Wiley & Sons, Inc. **2010**, pp. 505-533
4. **Tropsha, A**. QSAR in Drug Discovery. In: *Structure and Ligand-Based Drug Design*. Merz, K., Ringe, D., and Reynolds, C.L., Eds. Cambridge University Press, New York, **2010**, Chapter 10, pp. 151-164.
5. **Tropsha, A.,*** and Golbraikh, A. Predictive Quantitative Structure–Activity Relationships Modeling: Data Preparation and the General Modeling Workflow. In: *Handbook of Chemoinformatics Algorithms*, J.-L. Faulon and A. Bender, eds., Chapman and Hall, London., **2010**, Chapter 6, pp. 175-212.
6. **Tropsha, A.,*** and Golbraikh, A. Predictive Quantitative Structure–Activity Relationships Modeling: Development and Validation of QSAR Models. In: *Handbook of Chemoinformatics Algorithms*, J.-L. Faulon and A. Bender, eds., Chapman and Hall, London., **2010**, Chapter 7, pp. 213-233.
7. **Tropsha, A.** Complexity and Challenges of Modern QSAR Modeling and QSAR Based Virtual Screening, In Meyers, Robert (Ed.) Encyclopedia of Complexity and Systems Science. Springer New York. **2009**.
8. Varnek, A., **Tropsha, A**. (Eds) Chemoinformatics Approaches to Virtual Screening, RSC Publishing, Cambridge, UK, **2008** (also, Chapter 10 in this book by **Tropsha, A**. Application of Chemoinformatics Concepts in Structure Based Virtual Screening)

9. **Tropsha, A**.*, Wang, X.S. QSAR Modeling of GPCR ligands: Methodologies and Examples of Applications. Proc., Schering Foundation Res. Symp. Ser., Springer-Verlag, Berlin, **2007**, pp.49-74
10. **Tropsha, A.** Predictive QSAR (Quantitative Structure Activity Relationships) Modeling. In: Comprehensive Medicinal Chemistry II, V. 4 (Computer-Aided Drug Design), J. Mason, Ed., Elsevier, Oxford, UK, **2006**, pp. 149-165.
11. **Tropsha, A.** Variable Selection QSAR Modeling, Model Validation, and Virtual Screening. In: *Ann. Rev. Comp. Chem.*, Chapter 4, Y. Martin, Ed. , Elsevier, **2006**, Chapter 7, 113-126.
12. **Tropsha, A**. Application of Predictive QSAR Models to Database Mining. In: *Cheminformatics in Drug Discovery*, T. Oprea, Ed., Wiley-VCH, **2005**, pp. 437-455.
13. **Tropsha, A**.*, Carter, C.W., Jr., Cammer, S.A., Vaisman, I.I. Simplicial Neighborhood Analysis of Protein Packing (SNAPP): A Computational Geometry Approach to Studying Proteins. In: *Methods in Enzymology*, C.W. Carter Jr., Robert M. Sweet, Eds., Elsevier, **2003**, v. 374, pp. 509-544.
14. **Tropsha, A**.* Recent Trends in Quantitative Structure-Activity Relationships. In: *Burger's Medicinal Chemistry and Drug Discovery*, Abraham, D., Ed., Sixth Edition. Volume 1. New York: John Wiley & Sons, Inc. **2003**, pp. 49-77.
15. Cammer, S.A., Carter, C.W., **Tropsha, A.*** Identification of Sequence-Specific Tertiary Packing Motifs in Protein Structures using Delaunay Tessellation. In: *Computational Methods for Macromolecules: Challenges and Applications,* Proceedings of the 3rd International Workshop on Algorithms for Macromolecular Modeling, New York, Oct. 12-14, **2000**. Lecture Notes in Computational Science and Engineering (LNCSE), Vol. 24, pp. 477-494, Springer Verlag, Berlin, **2002**. Editors: T. Schlick and H. H. Gan.
16. **Tropsha, A.*** Rational Combinatorial Library Design and Database Mining using Inverse QSAR Approach. In: Combinatorial Library Design and Evaluation for Drug Discovery: Principles, Methods, Software Tools and Applications, A. K. Ghose and V. N. Viswanadhan, Eds, Chapter 12, Marcel Dekker, Inc., New York, **2001**, pp. 363-378.
17. **Tropsha, A**.,* and Zheng, W. Computer Assisted Drug Design. In: *Computational Biochemistry and Biophysics*, A. MacKerell Jr., O. Becker, B. Roux, M. Watanabe, Eds. Marcel Dekker, Inc., New York, **2001**, pp. 351-369.
18. **Tropsha, A.,*** and Cho, S. J. Cross-Validated R^2 Guided Region Selection for CoMFA Studies. In: 3D QSAR in Drug Design, H. Kubinyi, G. Folkers and Y. C. Martin, Eds., Volume III, Kluwer Academic Publishers, Spuiboulevard 50, P.O. Box 17, N-3300 AA Dordrecht, The Netherlands, **1998**, pp. 57-69.
19. **Tropsha, A.*** and Bowen, J.P. Molecular Modeling and Drug Design. In: Using Computers in Chemistry and Chemical Education, Zielinski, T.J. and Swift, M.L., Eds., ACS Book Series, ACS, **1997**, Chapter 17, pp. 309-330.
20. Mailman, R.B.,* Nichols, D.E., **Tropsha, A.** Molecular Drug Design and Dopamine Receptors. In: Dopamine Receptors, K. Neve and R. Neve, Eds. Humana Press, **1996**, pp. 105-133 (Invited review).
21. **Tropsha, A.,*** Yan, Y., Schneider, S.E., Li, L., and Erickson, B.W.* Relative Free Energies of Folding and Refolding of Model Secondary Structure Elements in Aqueous Solution. In Peptides: Chemistry, Structure, and Biology, R.S. Hodges and J.A. Smith, Eds. **1994**, pp. 883-885.

Refereed Papers/Articles:

1. **Tropsha A,** Bajorath J. Computational Methods for Drug Discovery and Design. *J Med Chem.* **2016** Jan 14;59(1):1. doi: 10.1021/acs.jmedchem.5b01945
2. Zakharov AV, Varlamova EV, Lagunin AA, Dmitriev AV, Muratov EN, Fourches D, Kuz'min VE, Poroikov VV, **Tropsha A**, Nicklaus MC. QSAR Modeling and Prediction of Drug-Drug Interactions. *Mol Pharm*. **2016** Jan 5. [Epub ahead of print]

3. Elkins JM, Fedele V, Szklarz M, Abdul Azeez KR, Salah E, Mikolajczyk J, Romanov S, Sepetov N, Huang XP, Roth BL, Al Haj Zen A, Fourches D, Muratov E, **Tropsha A**, Morris J, Teicher BA, Kunkel M, Polley E, Lackey KE, Atkinson FL, Overington JP, Bamborough P, Müller S, Price DJ, Willson TM, Drewry DH, Knapp S, Zuercher WJ. *Nat Biotechnol*. **2016,** 34(1):95-103**.**
4. Fourches D, Pu D, Li L, Zhou H, Mu Q, Su G, Yan B, Tropsha A. Computer-aided design of carbon nanotubes with the desired bioactivity and safety profiles. Nanotoxicology. **2015** Nov 2:1-10. [Epub ahead of print]
5. Low YS, Caster O, Bergvall T, Fourches D, Zang X, Norén GN, Rusyn I, Edwards R, **Tropsha A**.* Cheminformatics-aided pharmacovigilance: application to Stevens-Johnson Syndrome. *J Am Med Inform Assoc*. **2015** Oct 24. pii: ocv127. doi: 10.1093/jamia/ocv127. [Epub ahead of print]
6. Wambaugh JF, Wetmore BA, Pearce R, Strope C, Goldsmith R, Sluka JP, Sedykh A, **Tropsha A**, Bosgra S, Shah I, Judson R, Thomas RS, Woodrow Setzer R. Toxicokinetic Triage for Environmental Chemicals. *Toxicol Sci*. **2015**,;147(1):55-67
7. Fourches D, Muratov E, Tropsha A.. Curation of chemogenomics data. *Nat Chem Biol*. **2015** Jul 21;11(8):535
8. Alexander DL, **Tropsha** A, Winkler DA. Beware of R2: Simple, Unambiguous Assessment of the Prediction Accuracy of QSAR and QSPR Models. J Chem Inf Model. 2015 55(7):1316-22 PMID: 26099013.
9. Braga, R.C.,, Alves, V.M., Silva, M.F.B., Muratov, E., Fourches, D., Lião, L.M., Tropsha, A., and Andrade, C.H. Pred-hERG: A Novel web-Accessible Computational Tool for Predicting Cardiac Toxicity. Mol. Info, 2015, available online 7/20/2105 (DOI: 10.1002/minf.201500040)
10. Isayev, O., Fourches, D., Muratov, E,N,. Oses, C., Rasch K.M., **Tropsha, A.*,** and Curtarolo, S.* *Materials Cartography: Representing and Mining Materials Space Using Structural and Electronic Fingerprints. Chem. Mater., **2015**, 27: 735–743*. DOI: 10.1021/cm503507h
11. Fourches D, Politi R, **Tropsha A**.* Target-Specific Native/Decoy Pose Classifier Improves the Accuracy of Ligand Ranking in the CSAR 2013 Benchmark. *J Chem Inf Model*. **2015**, 55(1):63-71. doi: 10.1021/ci500519w
12. Baker, N.C., Fourches, D., **Tropsha, A**. Drug Side Effect Profiles as Molecular Descriptors for Predictive Modeling of Target Bioactivity. *Mol. Info*, **2015**, 34, 160-170.
13. Alves VM, Muratov E, Fourches D, Strickland J, Kleinstreuer N, Andrade CH, **Tropsha A**.* Predicting chemically-induced skin reactions. Part I: QSAR models of skin sensitization and their application to identify potentially hazardous compounds. *Toxicol Appl Pharmacol*. **2015** 284(2):262-72. doi: 10.1016/j.taap.2014.12.014.
14. Alves VM, Muratov E, Fourches D, Strickland J, Kleinstreuer N, Andrade CH, **Tropsha A**.* Predicting chemically-induced skin reactions. Part II. QSAR models of skin permeability and the relationships between skin permeability and skin sensitization. *Toxicol Appl Pharmacol*. **2015** 284(2):273-80 doi: 10.1016/j.taap.2014.12.013. PMCID: PMC4408226
15. Goldstein JI, Jarskog LF, Hilliard C, Alfirevic A, Duncan L, Fourches D, Huang H, Lek M, Neale BM, Ripke S, Shianna K, Szatkiewicz JP, **Tropsha A**, van den Oord EJ, Cascorbi I, Dettling M, Gazit E, Goff DC, Holden AL, Kelly DL, Malhotra AK, Nielsen J, Pirmohamed M, Rujescu D, Werge T, Levy DL, Josiassen RC, Kennedy JL, Lieberman JA, Daly MJ, Sullivan PF. Clozapine-induced agranulocytosis is associated with rare HLA-DQB1 and HLA-B alleles. *Nat Commun*. **2014** Sep 4;5:4757. doi: 10.1038/ncomms5757
16. Braga RC, Alves VM, Silva MF, Muratov E, Fourches D, **Tropsha A**, Andrade CH.* Tuning HERG out: antitarget QSAR models for drug development. *Curr Top Med Chem*. **2014**;14(11):1399-415

17. Blatt J,* Farag S, Corey SJ, Sarrimanolis Z, Muratov E, Fourches D, **Tropsha A**, Janzen WP. Expanding the scope of drug repurposing in pediatrics: the Children's Pharmacy Collaborative. *Drug Discov Today*. **2014** Nov;19(11):1696-8. doi: 10.1016/j.drudis
18. Politi R, Rusyn I, **Tropsha A**.* Prediction of binding affinity and efficacy of thyroid hormone receptor ligands using QSAR and structure-based modeling methods. *Toxicol Appl Pharmacol.* **2014**; 280(1):177-89. PMID: 25058446 [PubMed - as supplied by publisher]
19. Mu Q, Jiang G, Chen L, Zhou H, Fourches D, **Tropsha A**, Yan B.* Chemical basis of interactions between engineered nanoparticles and biological systems. *Chem Rev*. **2014** 114(15):7740-81.
20. Low, Y.S. Sedykh, A., Rusyn, I. and **Tropsha, A.*** Integrative Approaches for Predicting In Vivo Effects of Chemicals from their Structural Descriptors and the Results of Short-Term Biological Assays. *Curr. Top. Med. Chem*., **2014**, 14(11):1356-64.
21. Khashan, R., Zheng, W., **Tropsha, A**.* The Development of Novel Chemical Fragment-Based Descriptors Using Frequent Common Subgraph Mining Approach and Their Application in QSAR Modeling. Mol. Info, **2014**, 33, 201-215.
22. Thompson C, Sedykh A, Nicol M, Muratov E, Fourches D, **Tropsha A**, Kashuba A*. Cheminformatics Analysis to Identify Predictors of Antiviral Drug Penetration into the Female Genital Tract. *AIDS Res Hum Retroviruses*, **2014,** 30(11):1058-64
23. Luo M, Wang XS, Roth BL, Golbraikh A, **Tropsha A**.* Application of Quantitative Structure-Activity Relationship Models of 5-HT1A Receptor Binding to Virtual Screening Identifies Novel and Potent 5-HT1A Ligands. *J Chem Inf Model*. **2014,** 54(2):634-47.
24. Fourches D, Sassano MF, Roth BL, **Tropsha A**.* HTS navigator: freely accessible cheminformatics software for analyzing high-throughput screening data. *Bioinformatics*. **2014,** 30(4):588-589.
25. Cherkasov A, Muratov EN, Fourches D, Varnek A, Baskin II, Cronin M, Dearden J, Gramatica P, Martin YC, Todeschini R, Consonni V, Kuz'min VE, Cramer R, Benigni R, Yang C, Rathman J, Terfloth L, Gasteiger J, Richard A, **Tropsha A**.* QSAR Modeling: Where Have You Been? Where Are You Going To? *J Med Chem*. **2014** 57(12):4977-5010
26. Nile, A.H., Tripathi, A., Yuan, P., Mousley, C.J., Suresh, S., Wallace. I., Shah, S.D., Teotico-Pohlhaus D., Temple, B., Nislow, C., Giaever, G., **Tropsha, A**., Davis, R.W., St. Onge, R.W., and Bankaitis, V.A.* Chemical Inhibitors of Phosphatidylinositol Transfer Proteins Enable Highly Selective Interference With Specific Pathways of Phosphoinositide Signaling In Cells. *Nature Chem. Biol*, **2014,** 10(1):76-84.
27. Golbraikh A, Muratov E, Fourches D, **Tropsha A***. Data Set Modelability by QSAR. *J Chem Inf Model*. **2014,** 54(1):1-4.
28. Cern A, Barenholz Y, **Tropsha A**, Goldblum A.* Computer-aided design of liposomal drugs: In silico prediction and experimental validation of drug candidates for liposomal remote loading. *J Control Release*. **2014,** 173:125-31.
29. Fourches, D., **Tropsha, A**.* Using Graph Indices for the Analysis and Comparison of Chemical Datasets. *Mol. Info*, **2013**, 32, 827-842.
30. Zhang L, Fourches D, Sedykh A, Zhu H, Golbraikh A, Ekins S, Clark J, Connelly MC, Sigal M, Hodges D, Guiguemde WA, Guy RK, **Tropsha A**.* The Discovery of Novel Antimalarial Compounds Enabled by QSAR-based Virtual Screening. *J Chem Inf Model*. **2013**, 53, 475-92.
31. Fourches D, Muratov E, Ding F, Dokholyan NV, **Tropsha A**.* Predicting binding affinity of CSAR ligands using both structure-based and ligand-based approaches. *J Chem Inf Model*. **2013**, 53(8):1915-22.
32. May,E.,* Leitão, A., **Tropsha, A**., and Oprea, TI. A systems chemical biology study of malate synthase and isocitrate lyase inhibition in *Mycobacterium tuberculosis* during active and NRP growth. Comp. Bio. Chem., **2013,** 47, 167–180.

33. Zhang L, Sedykh A, Tripathi A, Zhu H, Afantitis A, Mouchlis VD, Melagraki G, Rusyn I, **Tropsha A**.* Identification of putative estrogen receptor-mediated endocrine disrupting chemicals using QSAR- and structure-based virtual screening approaches. *Toxicol Appl Pharmacol*. **2013**, 272, 67-76
34. Zhu XW, Sedykh A, Zhu H, Liu SS, **Tropsha A**.* The use of pseudo-equilibrium constant affords improved QSAR models of human plasma protein binding. *Pharm Res*. **2013**, 30(7):1790-8.
35. Yang K, Köck K, Sedykh A, **Tropsha A**, Brouwer KL.* An updated review on drug-induced cholestasis: mechanisms and investigation of physicochemical properties and pharmacokinetic parameters. *J Pharm Sci*. **2013**, 102(9):3037-57.
36. Sedykh A, Fourches D, Duan J, Hucke O, Garneau M, Zhu H, Bonneau P, **Tropsha A**.* Human Intestinal Transporter Database: QSAR Modeling and Virtual Profiling of Drug Uptake, Efflux and Interactions. *Pharm Res*. **2013,** 30(4):996-1007
37. Low Y, Sedykh A, Fourches D, Golbraikh A, Whelan M, Rusyn I, Tropsha A. Integrative chemical-biological read-across approach for chemical hazard classification. *Chem Res Toxicol.* **2013**, 26(8):1199-208.
38. Khashan R, Zheng W, **Tropsha A**.* Scoring protein interaction decoys using exposed residues (SPIDER): a novel multibody interaction scoring function based on frequent geometric patterns of interfacial residues. *Proteins*. **2012**, 80(9):2207-17.
39. Martin, T.; Harten, P.; Young, D.; Muratov, E.; Golbraikh, Al.; Zhu, H.; **Tropsha, A**.* Does Rational Selection of Training and Test Sets Improve the Outcome of QSAR Modeling?. *J Chem Inf Model*, **2012**, 52(10):2570-8.
40. **Tropsha, A**. Recent trends in statistical QSAR modeling of environmental chemical toxicity. *EXS*. **2012**;101:381-411.
41. Rusyn, I*, Sedykh, A., Low, Y., Guyton, K.Z., and **Tropsha, A**.* Predictive modeling of chemical hazard by integrating numerical descriptors of chemical structures and short-term toxicity assay data. *Tox. Sci*., **2012**, 127(1):1-9. PMC3327873
42. Hajjo R, Setola V, Roth BL, **Tropsha A**.* Chemocentric informatics approach to drug discovery: identification and experimental validation of selective estrogen receptor modulators as ligands of 5-hydroxytryptamine-6 receptors and as potential cognition enhancers. *J Med Chem*. **2012** Jun 28;55(12):5704-19. PMC3401608
43. Tang H, Wang XS,* Hsieh JH, **Tropsha A.*** Do crystal structures obviate the need for theoretical models of GPCRs for structure based virtual screening? Proteins. **2012**, 80(6):1503-21. PMID: 22275072
44. Lock EF, Abdo N, Huang R, Xia M, Kosyk O, O'Shea SH, Zhou YH, Sedykh A, **Tropsha A**, Austin CP, Tice RR, Wright FA, Rusyn I.* Quantitative high-throughput screening for chemical toxicity in a population-based in vitro model. *Toxicol Sci.* **2012,** 126(2), 578–588. PMC3307611
45. Proctor EA, Yin S, **Tropsha A**, Dokholyan NV*. Discrete molecular dynamics distinguishes native-like binding poses from decoys in difficult targets. *Biophys. J*., **2012** Jan 4;102(1):144-51. PMC3250674
46. Hsieh, J.-H., Yin, X., Wang, X.S., Liu, S., Dokholyan, N.V.,* and **Tropsha, A**.*. Cheminformatics Meets Molecular Mechanics: A Combined Application of Knowledge-Based Pose Scoring and Physical Force Field-Based Hit Scoring Functions Improves the Accuracy of Structure-Based Virtual Screening. . *J Chem Inf Model*. **2012** ;52(1):16-28. PMC3264743
47. Cern A, Golbraikh A, Sedykh A, **Tropsha A**, Barenholz Y,* Goldblum A*. Quantitative structure - Property relationship modeling of remote liposome loading of drugs. *J Control Release*. **2012,** 160, 147–157
48. Hsieh JH, Yin S, Liu S, Sedykh A, Dokholyan NV, Tropsha A. Combined application of cheminformatics- and physical force field-based scoring functions improves binding affinity prediction for CSAR data sets. *J Chem Inf Model*. **2011**; 51(9):2027-35. PMC3183266

49. Samarov D, Marron JS,* Liu Y, Grulke C, **Tropsha A**.* Local Kernel Canonical Correlation Analysis With Application To Virtual Drug Screening. *Ann Appl Stat*. **2011** Sep 1;5(3):2169-2196. PMCID: PMC3223065
50. **Tropsha, A**., Golbraikh, A., Cho, W.-J.* Development of kNN QSAR models for 3-arylisoquinoline antitumor agents. Bull. Korean Chem. Soc. **2011**;32(7):2397-2404.
51. Low Y, Uehara T, Minowa Y, Yamada H, Ohno Y, Urushidani T, Sedykh A, Muratov E, Kuz'min V, Fourches D, Zhu H, Rusyn I, **Tropsha A**.* Predicting Drug-Induced Hepatotoxicity Using QSAR and Toxicogenomics Approaches*. Chem Res Toxicol*. **2011**, 24(8):1251-62
52. Fleishman SJ et al (ca. 50 authors). Community-wide assessment of protein-interface modeling suggests improvements to design methodology. *J Mol Biol*. **2011** Nov 25;414(2):289-302
53. A.G. Artemenko, E.N. Muratov, V.E. Kuz'Min, N.N. Muratov, E.V. Varlamova, A.V. Kuz'Min, L.G. Gorb, A. Golius, F.C. Hill, J. Leszczynski* and **A. Tropsha***. QSAR analysis of the toxicity of nitroaromatics in Tetrahymena pyriformis: structural factors and possible modes of action. *SAR and QSAR Environ. Res*. **2011**, *22* (5-6), 1-27
54. Fourches D, Pu D, **Tropsha A.*** Exploring quantitative nanostructure-activity relationships (QNAR) modeling as a tool for predicting biological effects of manufactured nanoparticles. *Comb Chem High Throughput Screen*. **2011,** 14(3):217-25
55. Ebalunode JO, Zheng W, **Tropsha A**.* Application of QSAR and shape pharmacophore modeling approaches for targeted chemical library design. *Methods Mol Biol*. **2011**;685:111-33.
56. Oprea TI, May EE, Leitão A, **Tropsha A**.* Computational systems chemical biology. Methods *Mol Biol*. **2011**; **672**, 459-88.
57. Sedykh A, Zhu H, Tang H, Zhang L, Richard A, Rusyn I, **Tropsha A***. Use of in Vitro HTS-Derived Concentration-Response Data as Biological Descriptors Improves the Accuracy of QSAR Models of in Vivo Toxicity. *Environ Health Perspect*. **2011**, 119(3):364-70. PMID: 20980217
58. Sushko et al (38 authors total). Applicability Domains for Classification Problems: Benchmarking of Distance to Models for Ames Mutagenicity Set. *J. Chem. Info. Model*., **2010**, 50(12):2094-111
59. Hajjo R, Grulke CM, Golbraikh A, Setola V, Huang XP, Roth BL, **Tropsha A**.* Development, Validation, and Use of Quantitative Structure-Activity Relationship Models of 5-Hydroxytryptamine (2B) Receptor Ligands to Identify Novel Receptor Binders and Putative Valvulopathic Compounds among Common Drugs. J Med Chem. **2010** 11;53(21):7573-86
60. Walker, T., Grulke, C.M., Pozefsky, D., **Tropsha, A**. Chembench: A cheminformatics workbench. *Bioinformatics*, **2010**. 26(23):3000-1. PMCID: PMC2982152
61. Fourches, D., Pu, D., Tassa, C., Weissleder, R., Shaw, S.S., Mumper, R.J., **Tropsha, A**.* Quantitative Nanostructure Activity Relationship Modeling. ACS Nano, **2010**, 26;4(10):5703-12
62. Bandyopadhyay D, Huan J, Liu J, Prins J, Snoeyink J, Wang W, **Tropsha A**. Functional Neighbors: Inferring Relationships between Non-Homologous Protein Families Using Family-Specific Packing Motifs. *IEEE Trans Inf Technol Biomed*. **2010** Sep;14(5):1137-43.
63. **Tropsha, A**. Best Practices for QSAR Model Development, Validation, and Exploitation *Mol. Inf.,* **2010**, 29, 476 – 488
64. Fourches D, Muratov E, **Tropsha A**. Trust, But Verify: On the Importance of Chemical Structure Curation in Cheminformatics and QSAR Modeling Research. *J Chem Inf Model*. **2010**, 50, 1189–1204.
65. Williams, A.;* Tkachenko, V.; Lipinski, C.; **Tropsha, A**.; and Ekins, S. Free online resources enabling crowd-sourced drug discovery. *Drug Disc. World*, **2010**, 10, 33-39.

66. Rodgers AD, Zhu H, Fourches D, Rusyn I, Tropsha A.* Modeling Liver-Related Adverse Effects of Drugs Using kNearest Neighbor Quantitative Structure-Activity Relationship Method. *Chem Res Toxicol.* **2010**, 23(4):724-32. PMCID: PMC2965736
67. Fourches D, Barnes JC, Day NC, Bradley P, Reed JZ, **Tropsha A**.* Cheminformatics analysis of assertions mined from literature that describe drug-induced liver injury in different species. *Chem Res Toxicol*. **2010**, 23(1):171-83. (PMC2850112
68. Zhu H, Martin, T.M., Ye L, Sedykh, A., Young, D.M., **Tropsha, A**.* QSAR Modeling of Rat Acute Toxicity by Oral Exposure. *Chem. Res. Toxicol*., 2009, 22(12):1913-21
69. **Bandyopadhyay D**, Huan J, Prins J, Snoeyink J, Wang W, **Tropsha A**. Identification of family-specific residue packing motifs and their use for structure-based protein function prediction: II. Case studies and applications. *J Comput Aided Mol Des*. **2009**, 23(11):785-97.
70. **Bandyopadhyay D**, Huan J, Prins J, Snoeyink J, Wang W, **Tropsha A**. Identification of family-specific residue packing motifs and their use for structure-based protein function prediction: I. Method development. *J Comput Aided Mol Des*. **2009**, 23(11):773-84.
71. Zhu H, Ye L, Richard A, Golbraikh A, Wright FA, Rusyn I, **Tropsha A**. A novel two-step hierarchical quantitative structure-activity relationship modeling work flow for predicting acute toxicity of chemicals in rodents. *Environ Health Perspect*. **2009**, 117(8):1257-64. PMC2721870
72. Peterson, Y., Wang,, X.S., Casey, P.J., and **Tropsha, A**. Discovery of Geranylgeranyltransferase-I Inhibitors with Novel Scaffolds by the Means of Quantitative Structure-Activity Relationship Modeling, Virtual Screening, and Experimental Validation. *J. Med. Chem*., **2009**, 52(14):4210-20. PMCID: PMC2726652
73. Tang H, Wang XS, Huang XP, Roth BL, Butler KV, Kozikowski AP, Jung M, **Tropsha A**. Novel Inhibitors of Human Histone Deacetylase (HDAC) Identified by QSAR Modeling of Known Inhibitors, Virtual Screening, and Experimental Validation. *J Chem Inf Model*. **2009**, 49, 461-76.
74. **Ekins, S., Tropsha, A**. A turning point for blood-brain barrier modeling. *Pharm Res*. **2009** May;26(5):1283-4
75. Tetko IV*, Sushko I, Pandey AK, Zhu H, **Tropsha A**, Papa E, Oberg T, Todeschini R, Fourches D, Varnek A. Critical Assessment of QSAR Models of Environmental Toxicity against Tetrahymena pyriformis: Focusing on Applicability Domain and Overfitting by Variable Selection. *J Chem Inf Model*. **2008** 48(9):1733-46
76. Zhang, S., Kaplan, A., **Tropsha, A**.* HIV-1 Protease Function and Structure Studies with the Simplicial Neighborhood Analysis of Protein Packing (SNAPP) Method. *Proteins Struct. Func. Bioinf,* **2008** 73(3):742-753
77. Wang XS, Tang H, Golbraikh A, **Tropsha A**.***** Combinatorial QSAR Modeling of Specificity and Subtype Selectivity of Ligands Binding to Serotonin Receptors 5HT1E and 5HT1F. *J Chem Inf Model*. **2008**, 48(5):997-1013
78. Zhang L, Zhu H, Oprea T, Golbraikh A, **Tropsha A.*** QSAR Modeling of the Blood-Brain Barrier Permeability for Diverse Organic Compounds. *Pharm.Res*. **2008**, 25(8):1902-14.
79. Zhu H, **Tropsha A,*** Fourches D, Varnek A, Papa E, Gramatica P, Oberg T, Dao P, Cherkasov A, Tetko I V. Combinatorial QSAR Modeling of Chemical Toxicants Tested against Tetrahymena pyriformis. *J Chem Inf Model* **2008**; (48): 766-784
80. Hsieh JH, Wang XS, Teotico D, Golbraikh A, **Tropsha A**. Differentiation of AmpC beta-lactamase binders vs. decoys using classification kNN QSAR modeling and application of the QSAR classifier to virtual screening. *J Comput Aided Mol Des*. **2008** Sep;22(9):593-609
81. Zhu H, Rusyn I, Richard A, **Tropsha A**.* Use of cell viability assay data improves the prediction accuracy of conventional quantitative structure-activity relationship models of animal carcinogenicity. *Environ Health Perspect* **2008**; (116): 506-513. PMCID: PMC2291015

82. Karthikeyan,M.;* Krishnan,S.; Pandey,A.K.; Bender,A.; **Tropsha,A.** Distributed Chemical Computing using ChemStar: an Open Source Java Remote Method Invocation Architecture Applied to Large Scale Molecular Data from PubChem. *J.Chem.Inf.Model*., **2008**, 48 (4), 691-703
83. **Tropsha, A**.,* Golbraikh, A. Predictive QSAR Modeling Workflow, Model Applicability Domains, and Virtual Screening. *Curr. Pharm. Des*., **2007**, 13, 3494-3504.
84. Oprea TI,* **Tropsha A**, Faulon JL, Rintoul MD. Systems chemical biology. *Nat Chem Biol*. **2007**, 3, 447-50.
85. Zhang, S., Wei, L., Bastow, K., Zheng, W., Brossi, A., Lee, K.-H., **Tropsha, A**.* Application of validated QSAR models to database mining: discovery of novel tylophorine derivatives as potential anticancer agents. *J. Comp. Aid. Molec. Des*., **2007**, 21, 97-112.
86. Oprea, T.,* **Tropsha, A**. Target, Chemical and Bioactivity Databases – Integration is Key. *Drug Discov. Today*, **2006**, 3, 357-365
87. Votano JR,* Parham M, Hall LM, Hall LH, Kier LB, Oloff S, **Tropsha A**. QSAR modeling of human serum protein binding with several modeling techniques utilizing structure-information representation. *J Med Chem*. **2006**; 49,:7169-81.
88. Kozikowski AP, Roth B, **Tropsha A**. Why academic drug discovery makes sense. *Science*, **2006**, 313(5791), 1235-36
89. Zhang, S., Golbraikh, A., Oloff, S., Kohn, H., and **Tropsha, A**.* A Novel Automated Lazy Learning QSAR (ALL-QSAR) Approach: Method Development, Applications, and Virtual Screening of Chemical Databases using Validated ALL-QSAR Models. *J. Chem. Info. Mod*, **2006**, 46, 1984-95. PMCID: PMC2536695
90. Chen, X., **Tropsha, A**.* Calculation of the Relative Binding Affinity of Enzyme Inhibitors Using the Generalized Linear Response Method. *J. Chem. Theory. Comput*., **2006**, 2, 1435-1443.
91. Lima, P., Golbraikh, A., Oloff, S., Xiao, Y., **Tropsha, A.*** Combinatorial QSAR Modeling of P-Glycoprotein Substrates. *J. Chem. Info. Model*., **2006,** 46, 1245-1254.
92. Ghoneim OM, Legere JA, Golbraikh A, **Tropsha A,** Booth RG.***** Novel ligands for the human histamine H(1) receptor: Synthesis, pharmacology, and comparative molecular field analysis studies of 2-dimethylamino-5-(6)-phenyl-1,2,3,4-tetrahydronaphthalenes. *Bioorg Med Chem*. **2006**, 14, 6640-58.
93. Huan,J.; Bandyopadhyay,D.; Prins,J.; Snoeyink,J.; **Tropsha,A**.; Wang,W.* Distance-based identification of structure motifs in proteins using constrained frequent subgraph mining. *Comput. Syst. Bioinformatics. Conf*., **2006**, 227-238.
94. Bandyopadhyay, D., Huan, J., Wang, W., Snoeyink, J.,* Prins, J., and **Tropsha, A.*** Structure-based Function Inference Using Protein Family-Specific Fingerprints. *Protein Sci*., **2006**, 15, 1537–1543.
95. Zhang, S., Golbraikh, A., **Tropsha, A.*** The Development of Quantitative Structure-Binding Affinity Relationship (QSBR) Models Based on Novel Geometrical Chemical Descriptors of the Protein-Ligand Interfaces. *J. Med. Chem*., **2006**, 49, 2713-24.
96. Oloff, S., Zhang, S., Sukumar, N., Breneman, C., and **Tropsha, A**.* Chemometric Analysis of Ligand Receptor Complementarity: Identifying Complementary Ligands Based on Receptor Information (CoLiBRI). *J. Chem. Inf. Model.*, **2006**, 46, 844-851.
97. Huan, J., Bandyopadhyay, D., Wang, W.,* Snoeyink, J., Prins, J., and **Tropsha, A.*** Comparing Graph Representations of Protein Structure for Mining Family-Specific Residue-Based Packing Motifs. *J. Comp. Biol.*, **2005**, 12, 657–671.
98. Itskowitz, P., and **Tropsha, A**.* K Nearest Neighbors QSAR Modeling As a Variational Problem: Theory and Applications. *J. Chem. Inf. Model.*, **2005**, 45, 777-85.
99. Oloff, S., Mailman, R.B., and **Tropsha, A**.* Application of Validated QSAR Models of D1 Dopaminergic Antagonists for Database Mining. J. Med. Chem., **2005**, 48, 7322-32.

100.Medina-Franco, J.M., Golbraikh, A., Castillo, R., and **Tropsha, A**.* Quantitative Structure-Activity Relationship Analysis of Pyridinone HIV-1 Reverse Transcriptase Inhibitors Using the k Nearest Neighbor Method and QSAR-Based Database Mining. *J. Comput. Aided. Mol. Des*., **2005**, 19, 229–242.
101.Kovatcheva,A.; Golbraikh,A.; Oloff,S.; Feng,J.; Zheng,W.; **Tropsha, A**.* QSAR modeling of datasets with enantioselective compounds using chirality sensitive molecular descriptors. *SAR QSAR.Environ.Res.*, 2005, 16, 93-102.
102.Huan, J., Wang, W.,* Bandyopadhyay, D., Snoeyink, J., Prins, J., and Tropsha, A.* "Mining Family Specific Residue Packing Patterns from Protein Structure Graphs ". In: *Proceedings of the 8th Annual International Conference on Research in Computational Molecular Biology (RECOMB)*, pp. 308-315, 2004.
103.Votano JR,* Parham M, Hall LH, Kier LB, Oloff S, **Tropsha A**, Xie Q, Tong W. Three new consensus QSAR models for the prediction of Ames genotoxicity. Mutagenesis. 2004, 19, 365-77.
104.Ng C,* Xiao Y, Putnam W, Lum B, Tropsha A.* Quantitative structure-pharmacokinetic parameters relationships (QSPKR) analysis of antimicrobial agents in humans using simulated annealing k-nearest-neighbor and partial least-square analysis methods. J Pharm Sci. 2004, 93, 2535-44.
105.Xiao, Z., Varma, S., Xiao, Y.-D., Tropsha, A.* Modeling of p38 Mitogen-Activated Protein Kinase Inhibitors using the Catalyst HypoGen and k Nearest Neighbor QSAR Method. J. Mol. Graph. Mod., 2004, 23, 129-38.
106.Sherman, D.B., Zhang, S., Pitner, J.B., Tropsha, A.* Evaluation of the Relative Stability of Liganded vs. Ligand-Free Protein Conformations Using Simplicial Neighborhood Analysis of Protein Packing (SNAPP) Method. Proteins: Struct. Funct. Genet. 2004, 56, 828-838.
107.Edavettal, S.C., Carrick K, Shah R.R., Pedersen, L.C., Tropsha A., Pope, R..M, Liu, J.* A conformational change in heparan sulfate 3-O-sulfotransferase-1 is induced by binding to heparan sulfate. Biochem., 2004, 43, 4680-4688.
108.Shen, M., Beguin, C., Golbraikh, A., Stables, J., Kohn, H.,* and **Tropsha, A.*** Application of Predictive QSAR Models to Database Mining: Identification and Experimental Validation of Novel Anticonvulsant Compounds *J. Med. Chem.* **2004**, 47, 2356-64.
109.Sherman, D.B., Zhang, S., Pitner, J.B., **Tropsha, A.*** Evaluation of the Relative Stability of Liganded vs. Ligand-Free Protein Conformations Using Simplicial Neighborhood Analysis of Protein Packing (SNAPP) Method. *Proteins: Struct. Funct. Genet.* **2004**, 56, 828-838.
110.Kovatcheva, A., Golbraikh, A., Oloff, S., Xiao, Y., Zheng, W., Wolschann, P., Buchbauer, G., **Tropsha, A.** Combinatorial QSAR of Ambergris Fragrance Compounds. *J Chem. Inf. Comput. Sci.* **2004,** 44, 582-95.
111.Huan, J., Wang, W., Washington, A., Prins, J., Shah, R., **Tropsha, A.*** Accurate Classification of Protein Structural Families Using Coherent Subgraph Analysis. *Pacific Symposium on Biocomputing '04*, Hawaii, World Scientific, **2004**, 411-422.
112.Pendergraft III, W.F., Preston G.A., Shah, R., **Tropsha, A.,** Carter Jr., C.W., Jennette, J.C., & Falk, R.J.* Autoimmunity is triggered by cPR-3(105–201), a protein complementary to human autoantigen proteinase-3. *Nat. Med.*, **2003**, 10, 72-79.
113.Golbraikh, A., Shen, M., Xiao, Z., Xiao, Y., Lee, K.-H., and **Tropsha, A**.* Rational Selection of Training and Test Sets for the Development of Validated QSAR Models. *J. Comp. Aid. Mol. Design* **2003**, **17**, 241–253.
114.Krishnamoorthy, B. and **Tropsha, A.*** Development of a Four-Body Statistical Pseudo-Potential to Discriminate Native from Non-Native Protein Conformations. *Bioinformatics* **2003**, *19*, 1540-8.
115.Shen, M., Xiao, Y., Golbraikh, A., Gombar, V.K., and **Tropsha, A.*** An *In Silico* Screen For Human S9 Metabolic Turnover Using k-Nearest Neighbor QSPR Method. *J. Med. Chem*. **2003,** *46*, 3013-3020.

116.**Tropsha, A**.,* Gramatica. P.,* and Gombar, V.K.* The Importance of Being Earnest: Validation is the Absolute Essential for Successful Application and Interpretation of QSPR Models. *Quant. Struct. Act. Relat. Comb. Sci.* **2003**, *22*, 69-77.
117.Golbraikh, A., and **Tropsha, A**.* QSAR Modeling Using Chirality Descriptors Derived From Molecular Topology. *J Chem. Inf. Comput. Sci.* **2003**, *43*, 144-54.
118.Golbraikh, A., and **Tropsha, A**.* Predictive QSAR Modeling Based on Diversity Sampling of Experimental Datasets for the Test and Training Set Selection. *J. Comp. Aid. Mol. Design*, **2002**, *16***,** 357–369.
119.Shen, M. LeTiran, A., Xiao, Y. Kohn, H., and **Tropsha, A.*** QSAR Analysis of Functionalized Amino Acid Anticonvulsant Agents Using k-Nearest Neighbor and Simulated Annealing-PLS Methods. *J. Med. Chem*. **2002**, *45*, 2811-2823.
120.Xiao, Z., Xiao, Y., Feng, J., Golbraikh, A. **Tropsha, A.**,* and Lee, K.H.* Antitumor Agents. 213. Modeling of Epipodophyllotoxin Derivatives using Variable Selection k-Nearest Neighbor QSAR Method. *J. Med. Chem*. **2002**, *45*, 2294-2309
121.Golbraikh, A., and **Tropsha, A.*** Novel ZE-Isomerism Descriptors Derived from Molecular Topology and Their Application to QSAR Analysis. *J. Chem. Inf. Comput. Sci*. **2002**, *42*, 769-787.
122.**Tropsha, A.**, Zheng, W. Rational Principles of Compound Selection For Combinatorial Library Design. *Combi. Chem. & High Throughput Screen.* **2002**, *5*, 111-123.
123.Golbraikh, A. and **Tropsha, A.*** Beware of q^2! *J. Mol. Graphics Mod*. **2002**, *20*, 269-276.
124.Reynolds, C.H.,* **Tropsha, A.**,* Pfahler, L.B., Druker, R., Chakravorty, S., Ethiraj, G., Zheng, W. Comparison of the SAGE and SCA Algorithms for Diverse Selection of Structural Sublibraries using s- and u-Optimal Metrics. *J. Chem. Inf. Comput. Sci*. **2001**, *41*, 1470-1477.
125.Carter, C.W. Jr,* LeFebvre B.C., Cammer S.A., **Tropsha A**, Edgell, M.H. Four-body Potentials Reveal Protein-Specific Correlations to Stability Changes Caused by Hydrophobic Core Mutations. *J. Mol. Biol*. **2001**, *311*, 625-638.
126.**Tropsha, A**,* Zheng, W. Identification of the Descriptor Pharmacophores Using Variable Selection QSAR: Applications to Database Mining. *Current Pharm. Design*. **2001**, *7*, 599-612.
127.Pilger, C., Bartolucci, C., Lamba, D., **Tropsha, A.,*** and Fels, G.* Accurate Prediction of the Bound Conformation of Galanthamine in the Active Site of *Torpedo Californica* Acetylcholinesterase Using Molecular Docking. *J. Mol. Graphics. Mod.* **2001**, *19*, 288-296.
128.Golbraikh, A.,* Bonchev, D., Xiao, Y.-D., and **Tropsha, A.** Novel Chiral Topological Descriptors and Their Application to QSAR. // In: Rational Approaches to Drug Design. *Proceedings of the 13th European Symposium on Quantitative Structure-Activity Relationships*. 27 Aug – 1 Sept, 2000. Prous Science, 219-223.
129.Golbraikh, A., Bonchev, D., and **Tropsha, A.*** Novel Chirality Descriptors Derived from Molecular Topology, *J. Chem. Inf. Comput. Sci.* **2001**, *41*, 147-158.
130.Gan, H.H., **Tropsha, A.,** and Schlick, T.* Lattice Protein Folding with Two and Four-Body Statistical Potentials. *Proteins: Struct. Funct. Genet.* **2001**, *43*, 161-174.
131.Gan, H.H., **Tropsha, A.,** and Schlick, T.* Generating Folded Protein Structures with a Lattice Chain Algorithm. *J. Chem. Phys*. **2000**, *113*, 5511-5524.
132.**Tropsha, A.*** Recent Trends in Computer-Aided Drug Discovery. *Curr. Opinion in Drug Discovery and Development* **2000**, *3*, 310-313.
133.Xie, D., **Tropsha, A.**, and Schlick, T.* An Efficient Projection Protocol for Chemical Databases: Singular Value Decomposition with Truncated-Newton Minimization. *J. Chem. Inf. Comput. Sci.* **2000**, *40*, 167-177.
134.Zheng, W., and **Tropsha, A.*** A Novel Variable Selection QSAR Approach based on the K-Nearest Neighbor Principle. *J. Chem. Inf. Comput. Sci.* **2000**, 40, 185-194.

135. Zhang, S.-H., Feng, J., Kuo, S.-C., Brossi, A., Hamel, E., **Tropsha, A.*** and Lee, K.-H.* Antitumor Agents. 199. Three-Dimensional Quantitative Structure-Activity Relationship Study of the Colchicine Binding Site Ligands Using Comparative Molecular Field Analysis. *J. Med. Chem.* **2000**; *43*, 167-176.
136. Bucholtz, E.C., Booth, R.B., Wyrick, S.D., and **Tropsha, A.*** The Effect of Region Size on CoMFA Analyses. *Med. Chem. Res.* **1999***, 9,* 675-685.
137. Chen, X., Rusinko, A.R., III, **Tropsha, A.**, and Young, S.S.* Automated Pharmacophore Identification for Large Chemical Data Sets, *J. Chem. Inf. Comput. Sci.* **1999**, *39*, 887-896..
138. O'Connell, T.M., Wang, L., **Tropsha, A.**,* and Hermans, J.* The "random-coil" state of proteins: Comparison of database statistics and molecular simulations. *Proteins* **1999**, *36*, 407-418
139. Zheng, W., Cho, S.J., Waller, C.L., and **Tropsha, A.*** Rational Combinatorial Library Design. 3. Simulated Annealing Guided Evaluation (SAGE) of Molecular Diversity: A Novel Computational Tool for Diverse Library Design and Database Mining. *J. Chem. Inf. Comput. Sci.* **1999**, *39*, 738-746.
140. Bucholtz, E.C., Brown, R.L., **Tropsha, A.**,* Booth, R.B., and Wyrick, S.D.* Design, Synthesis, Evaluation and Comparative Molecular Field Analysis of Ligands for Histamine H_1 receptors. *J. Med. Chem.* **1999**, *42*; 3041-3054.
141. Hoffman, B.T., Cho, S. J., Zheng, W., Wyrick, S., Nichols, D. E., Mailman, R. B.; **Tropsha, A.*** QSAR Modeling of Dopamine D_1 Agonists using Comparative Molecular Field Analysis, Genetic Algorithms-Partial Least Squares, and K Nearest Neighbor Methods. *J. Med. Chem.* **1999**, *42*, 3217-3226.
142. Chen, X. and **Tropsha, A.*** Calculation of the hydration free energies using an extended linear response method. *J. Comp. Chem.* **1999**, *20*, 749-759*.*
143. **Tropsha, A.**,* Cho, S. J., and Zheng, W. "New Tricks for an Old Dog": Development and Application of Novel QSAR Methods for Rational Design of Combinatorial Chemical Libraries and Database Mining. In: *Rational Drug Design: Novel Methodology and Practical Applications*, Parrill, A.L. and Reddy, M.R., Eds, ACS Symposium Series No 719, **1999**, pp. 198-211.
144. Vaisman, I.I.,* **Tropsha, A.**, and Zheng, W. Compositional Preferences in Quadruplets of Nearest Neighbor Residues in Protein Structures. In: *"Intelligence and Systems"*, Proc. of IEEE Int. Symp., Washington, 1998, pp. 163-168.
145. Zheng, W., Cho, S.J., and **Tropsha, A.*** Rational Design of a Targeted Combinatorial Chemical Library with Opiate-like Activity. *Int. J. Quant. Chem*. **1998**, *69*, 65-75.
146. Shi, Q., Chen, K., Chen, X., Brossi, A., Verdier-Pinard, P., Hamel, E., McPhail, A. T., **Tropsha, A.**,* Lee, K.-H.* Antitumor Agents. 183. Syntheses, Conformational Analyses, and Antitubulin Activity of Allothiocolchicinoids, *J. Org. Chem*. **1998,** *63*, 4018-4025.
147. Cho, S.J., Zheng, W., and **Tropsha, A.*** Rational Combinatorial Library Design. 2. Rational Design of Targeted Combinatorial Peptide Libraries Using Chemical Similarity Probe and the Inverse QSAR Approaches. *J. Chem. Inf. Comput. Sci.* **1998**, *38*, 259-268.
148. Zheng, W., Cho, S.J., and **Tropsha, A.*** Rational Combinatorial Library Design. 1. FOCUS-2D: A New Approach to the Design of Targeted Combinatorial Chemical Libraries. *J. Chem. Inf. Comput. Sci.* **1998**, *38*, 251-258..
149. Mansfield, S.G., Cammer, S., Alexander, S.C., Muehleisen, D.P., Gray, R.S., **Tropsha, A.,*** and Bollenbacher, W.E.* Molecular cloning and characterization of an invertebrate cellular retinoic acid binding protein. *Proc Natl Acad Sci U S A* **1998**, *95*, 6825-6830.
150. Cho, S.J., Zheng, W., and **Tropsha, A.*** Focus-2D: A New Approach to the Design of Targeted Combinatorial Chemical Libraries. *Pacific Symposium on Biocomputing '98*, Hawaii, Jan. 4-9, 1998. Eds. R.B. Altman, A.K. Dunker, L. Hunter and T.E. Klein, World Scientific, Singapore, 1998, pp. 305-316.

151.Cho, S.J., Serrano, M.G., Bier, J. and **Tropsha, A.*** Structure Based Alignment and Comparative Molecular Field Analysis of Acetylcholinesterase Inhibitors. *J. Med. Chem.* **1996**, *39*, 5064-5071.

152.Zheng, W., Cho, S.J,. Vaisman, I.I., and **Tropsha A.*** A New Approach to Protein Fold Recognition Based on Delaunay Tessellation of Protein Structure. In: *Pacific Symposium on Biocomputing '97*, Hawaii, Jan. 6-9, 1997, Eds. L. Hunter and T.E. Klein, World Scientific, Singapore, 1997, pp. 486-497.

153.Wang, L., O'Connell, T., **Tropsha, A.*** and Hermans J.* Molecular Simulations of β-sheet twisting. *J. Mol. Biol*. **1996**, *262*, 283-293.

154.Cho, J., **Tropsha, A.**,* Suffness, M. & Lee, K.-H.* Antitumor Agents. 163. Three-Dimensional QSAR Study of 4'-*O*-Demethylepipodophyllotoxin Analogs Using the CoMFA/q^2-GRS Approach. *J. Med. Chem*. **1996**, *39*, 1383-1395.

155.Singh, R.K., **Tropsha, A.**, and Vaisman, I.I.,* Delaunay Tessellation of Proteins: Four Body Nearest Neighbor Propensities of Amino Acid Residues. *J. Comput. Biol.* **1996**, *3*, 213-222.

156.Singh, R.K., Hoffman, D.L., and **Tropsha, A.*** Rapid Comparison and Classification of Protein 3D Structures using One-Dimensional Structure Profiles. In: *Pacific Symposium on Biocomputing '96*, Hawaii, Jan. 3-6, 1996, L. Hunter and T.E. Klein, Eds. World Scientific, Singapore, **1995**, pp. 743-744.

157.**Tropsha, A.**,* Singh, R.K., Vaisman, I.I., and Zheng, W. Statistical Geometry Analysis of Proteins: Implications for Inverted Structure Prediction. In: *Pacific Symposium on Biocomputing '96* Hawaii, Jan. 3-6, 1996, L. Hunter and T.E. Klein, Eds. World Scientific, Singapore, **1995**, pp. 614-623.

158.Wang, L., O'Connell, T., **Tropsha, A.*** and Hermans J.* Energetic Decomposition of the α-Helix-Coil Equilibrium of a Dynamic Model System. *Biopolymers* **1996**, *39*, 479-489.

159.Mottola, D.M., Laiter, S., Watts, V.J., **Tropsha, A**.,* Wyrick, S.W., Nichols, D.E., & Mailman, R.* Conformational Analysis of D_1 Dopamine Receptor Agonists: Pharmacophore Assessment and Receptor Mapping. *J. Med. Chem*. **1996**, *39*, 285-296.

160.Hoffman, D., Laiter, S., Singh, R.K. Vaisman, I.I., and **Tropsha, A**.* Rapid Protein Structure Classification Using One-Dimensional Structure Profiles on the BioSCAN Parallel Computers. *CABIOS* **1995**, *11*, 675-679.

161.Wang, L., O'Connell, T., **Tropsha, A**.*, and Hermans, J.* Thermodynamic parameters for the helix-coil transition of oligopeptides: molecular dynamics simulation with the peptide growth method. *Proc. Natl. Acad. Sci. USA* **1995**, *92*, 10924-10928.

162.Laiter S., Hoffman, D., Singh, R., Vaisman, I.I., and **Tropsha, A**.* Pseudotorsional OCCO Backbone Angle as a Single Descriptor of Protein Secondary Structure. *Protein Sci.* **1995**, *4*, 1633-1643.

163.Yan, Y., Erickson, B.W., and **Tropsha, A**.* Free Energy for Folding and Refolding of Four Types of Beta Turns: Simulation of the Role of D/L Chirality. *J. Am. Chem. Soc*., **1995**, *117*, 7592-7599.

164.Cho, S. J. and **Tropsha, A**.* Cross-Validated R^2 Guided Region Selection for Comparative Molecular Field Analysis (CoMFA): A Simple Method to Achieve Consistent Results. *J. Med. Chem.* **1995**, *38*, 1060-1066.

165.Chen, X. and **Tropsha, A**.* Relative Binding Free Energies of the HIV-1 Protease Peptide Inhibitors: The Role of the Active Site Protonation State. *J. Med. Chem.* **1995***, 38*, 42-48.

166.Krishnaswami, K., **Tropsha, A**.* & Smith, P.C.* Semiempirical Calculations of Intramolecular Acyl Transfer in Cis-enols of O-aroyl Acetylacetones. *THEOCHEM* **1995**, *332*, 85-91.

167.Vaisman, I.I.,* Brown, F.K., & **Tropsha, A**. Distance Dependence of Water Structure Around Model Solutes. *J. Phys. Chem*. **1994**, *98*, 5559-5564.

168.Zhang, Y., **Tropsha, A**., McPhail, A.T., Lee, K.-H.* Antitumor Agents. 142. *In Vitro* Inhibitory Activity of Etoposide Derivative NPF Against Human Tumor Cell Lines and a Study of its Conformation by X-Ray Crystallography, Molecular Modeling, and NMR Spectroscopy. *J. Med. Chem*. **1994**, *37*, 1460-1464.

169.Rozzelle, J., **Tropsha A.***, and Erickson B.W.* Rational Design of a three-heptad coiled coil protein and comparison by molecular dynamics simulation with the GCN4 coiled coil: Presence of interior three-center hydrogen bonds. *Protein Sci*. **1994**, *3*, 345-355

170.Chen, X., Bartolotti, L., Ishaq, K., and **Tropsha, A**.* Molecular Simulation of Alkyl Boronic Acids: Molecular Mechanics and Solvation Free Energy Calculations. *J. Comp. Chem*. **1994**, *15*, 333-345.

171.Edgerton, M.D., **Tropsha, A.**,* and Jones, A.M.* The Auxin-Binding Site of Auxin-Binding Protein 1. *Phytochem.* **1994**, *35*, 1111-1123.

172.Yan, Y., **Tropsha, A.**,* Hermans, J., and Erickson, B.W.* Free Energies for Refolding of the Common beta turn into the inverse-common beta turn: Simulation of the Role of D/L Chirality. *Proc. Natl. Acad. Sci. USA* **1993**, *90*, 7892-7902.

173.**Tropsha, A.**,* Kizer, J. S., and Chaiken, I. M. Making Sense from Antisense: A Review of Experimental Data and Developing Ideas on Sense-Antisense Peptide Recognition. *J. Mol. Recognit.* **1992**, *5*, 43-54.

174.**Tropsha, A.**, and Hermans, J.* Application of Free Energy Simulations to the Binding of a Transition-State-Analog Inhibitors to HIV Protease. *Protein Engng.* **1992**, *5*, 29-33.

175.**Tropsha, A.**,* Bowen, J. P. Brown, F. K., and Kizer, J. S. Do Interhelical Hydrogen Bonds Participate in the Formation of Leucine Zipper Coiled Coils?. *Proc. Natl. Acad. Sci. USA* **1991***, 88*, 9488-9492.

176.Kizer, J.S.*, and **Tropsha, A.** A motif found in propeptides and prohormones that may target them to secretory vesicles. *Biochem. Biophys. Res. Com.* **1991**, *174*, 586-592.

177.**Tropsha, A. E.,** Nizhny, S. V., and Yaguzhinsky, L. S.* Structure - Activity Relationships in Series of Antagonists of Muscarinic Acetylcholine Receptor: Four Modes of Antagonist - Receptor Binding. *Bioorgan. Chem., USSR*, **1986**, *11*, 748-761.

178.**Tropsha, A.** E., Nizhny, S. V., and Yaguzhinsky, L. S.* Structure - Activity Relationships in Series of Agonists of Muscarinic Acetylcholine Receptor: Three types of Agonist Receptor Binding. *Bioorgan. Chem. USSR*, **1986**, *11*, 737-747.

179.Tsybulskaya, M.V. Antonenko, Yu. N., **Tropsha, A.** E., and Yaguzhinsky, L.S.* Thyroid Hormones as Dipole Modifiers of the Phospholipid Membranes. *Biophyzika USSR*, **1984**, *29*, 801-805.

180.**Tropsha, A. E.**, Rakhmaninova, A. B., and Yaguzhinsky, L. S.* Configuration and Properties of the Thyroid Hormones Binding Site at the Specific Receptor. *Bioorgan. Chem. USSR,* **1984**, *10*, 483-492.

Invited Oral Presentations

INVITED LECTURES AND SEMINARS:

Dec. 2015	Pacifichem, Honolulu, HI. *Materials Informatics for Materials Design*
Dec. 2015	JAMIA Journal Club (Webinar). *Cheminformatics-aided pharmacovigilance: application to Stevens-Johnson Syndrome*
Nov. 2015	Russian American Science Association annual meeting, Washington, DC. *Trust, but verify: on the importance of experimental data curation*
Oct. 2015	European Bioinformatics Institute, Hingxton, UK. *Development and interpretation of ADMET QSAR models with hybrid descriptors combining computed and*

experimental molecular properties

Aug. 2015 250th ACS Meeting. Boston, MA. *Alerting about toxicity alerts*.

Aug. 2015 250th ACS Meeting. Boston, MA. *Integrated use of chemical and biological descriptors improves the accuracy and interpretability of toxicity prediction models*.

Aug. 2015 250th ACS Meeting. Boston, MA.*What it takes to develop trust/worthy models*.

Apr 2015 University of Michigan, Ann Arbor, MI. *On the importance of data (and model!) curation in molecular modeling*

Apr. 2015 University of Buffalo, Rosewell Park. *Rational Drug Design*

Mar. 2015 Cosmetics Europe Workshop, Brussels, Belgium. *Computational molecular modeling of chemical safety enriched by the use of molecular docking or short-term biological screening assays*

Dec. 2014 Aramco, Boston. *Quantitative Structure-Property Relationships (QSPR)*

Dec. 2014 46th Annual Sympsium of the Society of Toxicology of Canada, Ottawa, Canada. Hybrid Chemical-Biological Approaches to Toxicity Prediction

Nov. 2014 International Cheminformatics Conference, Kazan. Russia. *Current trends in QSAR modeling.*

Nov. 2014 Indo-US Conference on Molecular Modeling and Informatics in Drug Design, S.A.S. , Punjab, India. *Cheminformatics Approaches to Drug Discovery: Challenges, Solutions, and Opportunities*.

Nov. 2014 NanoDDS, Chapel Hill, NC. *Computer Modeling of Nanomaterials and Liposome-based Drug Delivery Systems*

Oct. 2014 Medical University of Lublin, Lublin, Polans. *Cheminformatics Approaches to Drug Discovery: Challenges, Solutions, and Opportunities*.

Sep. 2014 EuroQSAR, St. Petersburg, Russia. *Alerting About Single Alerts: Bridging SAR and QSAR Approaches for Flagging or Avoiding Compounds with Undesired Toxicity Profiles*

Aug. 2014 American Chemical Society Meeting, San Francisco, US. Materials Cartography (Awarded as best presentation at the Emerging Technologies Symposium)

June 2014 Chemoinformatics Strasbourg Summer School, Strasbourg, France. *On the use of biological descriptors of chemical compounds to enrich traditional cheminformatics applications*

April 2014 Russian Cultural Center, Washington, DC *Cheminformatics: from Mendeleev to our time*

April 2014 Univesity of Buffalo, Buffalo, NY. *Computational Modeling of Molecular Bioactivity for Guiding the Experimental Design of Novel Bioactive Compounds*

Jan. 2014 FutureTox Conference, Chapel Hill, NC. *QSAR in Predictive Toxicology*.

Dec. 2013 US-EU CoR1 meeting, Washington, DC. *Nanomaterials Registry*

Sep. 2013 American Chemical Society Meeting, Indianapolis, IN. *QSAR Modeling on the Web. ChemBench: Free Online QSAR Modeling Tool*

Sep. 2013 EuroTox 2013 Congress, Interlaken, Switzerland. *Potential of Short-Term Biological Assays to Quantitatively Predict Chronic Toxicity*

Aug. 2013 Kazan Summer School on Chemoinformatics, Kazan, Russia. *SAR/QSAR Modeling: State of the Art.*

July 2013 Gordon Reseach Confrence on Computer-Assisted Drug Discovery. *What to expect when you're expecting...and editorial decision on your manuscript?*

June 2013 University of Chicago. *Contrasting and Combining Ligand Based and Structure Based Strategies for Computational Drug Discovery*

May 2013 Workshop on Computer-Aided Drug Design, Siena, Italy. *Best Practices and New Applications of QSAR Modeling.*

Feb. 2013 St. Jude's Children Hospital, Memphis, TN. *Predictive QSAR Models Help Identify Novel Bioactive Molecules*

Sep. 2012 Annual meeting of the European Federation for Medicinal Chemistry, Berlin, Germany. *Improved Prediction of in vivo Effects by Combining Cheminformatics and Short-term Assay Data*.

Aug. 2012 Institute of Bioinformatics and Applied Biotechnology, Helmholtz Zentrum, Munich. *Experiment-Assisted Computational Drug Discovery.*

Aug. 2012 EuroQSAR, Vienna, Austria. *QSAR Without Borders (but not without boundaries).*

June 2012 Third Strasbourg Summer School on Chemoinformatics, Strasbourg, France. *Experiment-Assisted Computational Drug Discovery*.

June 2012 14th International Environmental QSAR meeting, Tallin, Estonia. *Environmental QSAR Modeling: Where have you been, where are you going?*

Apr 2012 Boehringer Ingelheim, Ridgefield, CT. *Integrating chemical and biological data streams to improve accuracy and interpretability of ADMET models*

Mar 2012 National meeting of the American Chemical Society. *Experiment-Assisted Computational Drug Discovery*

Mar 2012 National Center for Translational Technologies, NIH. *Challenges and solutions for modeling chemical genomics data streams: chemical structure – in vitro – in vivo extrapolation*

Jan. 2012 SRC Metrology Webinar Series: *Quantitative Nanostructure-Activity Relationships (QNAR) modeling: Applications to Rational Design of Nanomaterials with the Desired Bioactivity Profile*

Jan. 2012 European Bioinformatics Institute, Hinxston, UK: *Many Challenges and Some Solutions for Modeling Chemical Genomics Data: navigating structure – in vitro – in vivo response data space*

Jan. 2012 Dow Chemicals, Midland, MI: *Cheminformatics Tools for Toxicity Prediction*

Dec. 2011 Nanoinformatics Conference, Arlington, DC: *Quantitative Nanostructure-Activity Relationships (QNAR) modeling: Applications to Rational Design of Nanomaterials with the Desired Bioactivity Profile*

Nov. 2011 Univ. of Strasbourg. Quantitative Nanostructure-Activity Relationships (QNAR) modeling: Applications to Rational Design of Nanomaterials with the Desired Bioactivity Profile

Nov. 2011 Massaryk University, Brno, Czech Republic. Experiment-Assisted Computational Drug Discovery

Oct. 2011 SERMACS 2011: Experiment-Assisted Computational Drug Discovery

Sep. 2011 ECHA, Helsinki, Finland: Cheminformatics Tools for Toxicity Prediction

Sep. 2011 Joint Research Center of European Commission, Ispra, Italy: Cheminformatics Tools for Toxicity Prediction

Sep. 2011 NAS: Applying 21st Century Toxicology to Green Chemical and Material Design

Aug. 2011 EPA, Washington, DC. Cheminformatics Tools for Toxicity Prediction

Jun. 2011 SRC/University of Arizona Webinar. Computer-Aided Design

of Nanomaterials with the Desired Bioactivity and Safety Profiles

Apr. 2011 European Commission COST workshop on QNTR, Maastricht, Netherlands. *Quantitative Nanostructure-Activity Relationships (QNAR) models as tools for predicting biological effects of manufactured nanoparticles*

Mar. 2011 Bar Ilan University, Ramat Gan, Israel. *Experiment-Assisted Computational Discovery of Biological Active Substances: From Medicinal Agents to Nanomaterials.*

Mar. 2011 University of Cyprus, Nicosia, Cyprus. *Cheminformatics Analysis of Bioactive Compounds to Establish Predictive Structure-Activity Relationships.*

Feb. 2011 School of Pharmacy, Hebrew University of Jerusalem, Israel. *Experiment-Assisted Computational Drug Discovery.*

Feb. 2011 Annual meeting of the Israeli Chemical Society, Tel Aviv, Israel. *Novel Cheminformatics Approaches to Chemical Toxicity Prediction.*

Dec. 2010 PACIFICHEM, Honolulu, Hawaii. *Quantitative Nanostructure – Activity Relationships*

Oct. 2010 Medical University of South Carolina, Charlestone, SC. *Chemocentric Informatics: Computational Analysis of Integrated Chemical-Biological Data Sources to Enable Molecular Probe and Drug Discovery*

Oct. 2010 Univ. Of Missouri, Columbia, Missouri. *Changing the Paradigm: Experiment-Assisted Computational Drug Discovery*

Sep. 2010 13th EuroQSAR, Rhodos, Greece. *Novel Approaches to Chemical Toxicity Prediction Relying on the Entire Structure – in vitro – in vivo Data Continuum*

Sep. 2010 GlaxoSmithKline, Stevanage, UK. *Mining PubMed and other databases for chemical-target-disease associations: What a MeSH*!

Sep. 2010 2nd International LHASA Symposium on Horizos inToxicty Prediction, Leeds, UK. *Good Practices for Building Robust QSAR Models of Chemical Toxicity*

Sep. 2010 ICES, Singapore. Mini-Workshop on*: Best practices for developing predictive QSAR models*

Sep. 2010 National University of Singapore, 1st Medicinal Chemsitry Symposium. *Novel Approaches to Predictive ADME/Tox Modeling Integrating Chemical Deescriptors and Short-term Biological Assay Data*

Aug. 2010 Fall 2010 ACS meeting, Boston, MA. Cheminformatics meets molecular mechanics: a combined application of knowledge based pose scoring and physical force field-based hit scoring functions improves the accuracy of virtual screening

Aug. 2010 Fall 2010 ACS meeting, Boston, MA. Chemocentric informatics: Enabling bioactive compound discovery through structural hypothesis fusion

June 2010 3rd Workshop Chemoinformatics in Europe: Research and Teaching, Obernai, France. *Best practices for developing predictive QSAR models*.

Apr.2010 Annual meeting of Severe Adverse Effects Consortium/Drig Induced Liver Injury Network (SAEC/DILIN), Durham, NC. *Cheminformatics approaches to hepatotoxicity prediction*

Apr.2010 University of Houston, Houston, TX. *Accurate Prediction of Biological Activity from Chemical Structure.*

Mar.2010 TACBAC 2010, Hinxton, UK. Hinxton, UK. *Integrated Informatics Approaches toward Small Molecule Biological Probe and Drug Discovery*

Dec.2009 University of Minnesota, Minneapolis, MN. *Integrated Informatics Approaches*

toward Small Molecule Biological Probe and Drug Discovery

Nov.2009 Univ. Louis Pasteur, Strasbourg, France. *Predictive QSAR Modeling of Animal Toxicity Endpoints Using a Combination of Chemical and Biological Descriptors of Molecules*

Nov. 2009 University of Illinoice in Chicago, Chicago, US. *Identification of Family-Specific Residue Packing Motifs and their use for Structure-Based Protein Function Prediction*

Oct. 2009 18th Conference on Current Trends in Computational Chemistry (CCTCC), Jackson, MS. *Predictive QSAR Modeling of Animal Toxicity Endpoints Using a Combination of Chemical and Biological Descriptors of Molecules*

Oct. 2009 BCB Training Program, UNC-CH. *Protein function prediction using structural motif-based approaches*

Oct.2009 Hamner Institute, RTP, NC. *Are in vitro data useful for predicting chemical toxicity?*

Sep.2009 OpenTox Meeting, Rome, Italy. *Collaborative QSAR Modeling of Ames Mutagenicity: "All for One and One for All"*

Sep. 2009 Molecular Modeling Conference, Erlangen, Germany. *Chem(o)informatics exploration of the entire biological data continuum for building predictive chemical toxicity models*

Sep. 2009 NAS workshop on Computational Toxicology, Washington, DC. *Combining High Throughput Screening Data and QSAR Modeling to Improve Hazard Predictions*

Aug.2009 Fall 2009 ACS Meeting, Washington, DC. *Trust but Verify: On the importance of experimental data curation prior to building (Q)SAR models*

July 2009 MACC-3 International Conference, Odessa, Ukraine. *Prediction of Animal Toxicity Endpoints Using a Combination of Chemical and in vitro Biological Descriptors of Molecules*

June 2009 CCG User Group Meeting, Montreal, Canada. *Combining Text Mining and QSAR Modeling for Bioactivity Prediction*

June 2009 CADD conference, Montreal, Canada. *Enabling the Experimental Hit Discovery by Predictive QSAR Modeling and Virtual Screening*

May 2009 University of Munich, Munich, Germany. *Protein function prediction using structural motif-based approaches*

May 2009 ToxCast Summit, RTP, NC, USA. *Prediction of animal toxicity endpoints of ToxCast Phase I compounds using a combination of chemical and biological in vitro descriptors*

May 2009 27th Noordwijkerhout-Camerino-Cyprus Conference, Noordwijkerhout, the Netherlands. *The QSARome of the GPCRome.*

May 2009 Molecular Modeling Workshop, Siena, Italy. Best practices for developing predictive QSAR models.

Apr.2009 CHI Life Sciences Conference, Boston, MA. *Cheminformatics Analysis of Literature Assertions Describing Drug-Induced Liver Injury*

Mar.2009 Spring 2009 ACS meeting, Salt Lake City, UT. *Assessing the Biological Effects of Nanoparticles Using Quantitative Nanostructure – Activity Relationships*

Mar.2009 Carolina Center for Genome Sciences, Chapel Hill, NC. *Cheminformatics Approaches To Drug Discovery*

Feb.2009 School of Information and Library Science, UNC-CH. *The use of Informatics*

Approaches in Cheminformatics.

Dec. 2008 Il Congreso De Fisicoquimica Teorica Y Computacional, Choroni, Venezula. Predictive QSAR Modeling and Virtual Screening.

Dec. 2008 University of Venezuela, Caracas, Venezuela. *The good practices for developing robust QSAR models*

Nov. 2008 4th German Cheminformatics Conference, Goslar, Germany. *Graph representation of molecular datasets*.

Oct. 2008 Cheminfo, Bryn Mawr, PA. *A Combined Use of In Vitro Screening and Cheminformatics Approaches Improves the Accuracy of In Vivo Toxicity Prediction for Environmental Molecules*

Oct. 2008 Cheminfo, Bryn Mawr, PA. *Cheminformatics Analysis of Polypharmacological Databases*

Sep. 2008 University of Cambridge, UK. *Representation and Predictive Modeling of Complex Biomolecular Databases*

Sep. 2008 13th EuroQSAR meeting, Uppsala, Sweden. *A Combined Use of In Vitro Screening and Cheminformatics Approaches Improves the Accuracy of In Vivo Toxicity Prediction for Environmental Molecules*

Sep. 2008 US EPA, RTP, NC. *A Combined Use of In Vitro Screening and Cheminformatics Approaches Improves the Accuracy of In Vivo Toxicity Models*

Aug. 2008 227th Meeting of the American Chemical Society, Philadelphia, PA. *Modeling of Complex Chemical Genomics Databases*

June 2008 University of Bonn, Germany. *Biomolecular Structure-Function Relationships and Structure Based Function Prediction*

June 2008 2nd Workshop: Chemoinformatics in Europe: Research and Teaching, Obernai, France. *The good, the bad, and the ugly…practices of QSAR modeling*

Mar 2008 Society of Toxicology, Annual Meeting, Seattle, WA. *Modeling Toxicity from High Throughput Screening Data on Environmental Chemicals*

Mar 2008 University of British Columbia, Vancouver, CA. *Cheminformatics Approaches to Drug Discovery*

Feb. 2008 Boehringer Ingelheim, Ridgefield, CT. *Challenges and Solutions for Building Experimentally Validated QSAR Models*

Feb. 2008 Univ. Louis Pasteur, Strasbourg, France. *Recent Advances in QSAR Modeling*

Jan. 2008 Pfizer, Inc, St. Louis. *Cheminformatics-based Decision Support for Biological Screening of Chemical Compounds*

Nov. 2007 Boehringer Ingelheim, Montreal, Canada. *Predictive QSAR Modeling Enables the Experimental Discovery of Biologically Active Molecules*.

Nov. 2007 3rd Annual Conference of German Chemoinformatics and QSAR Society, Goslar, Germany (after dinner speaker). *The Cheminformatics Manifesto*.

Sep. 2007 ACS Prospectives, San Francisco, CA. *Cheminformatics Approaches to Virtual Screening.*

Sep. 2007 CMPTI, Moscow, Russia. *Combinational QSAR Modeling of Chemical Toxicants Tested Against Tetrahymena Pyriformis.*

Sep. 2007 ACS meeting, Boston, MA. *Frequent common subgraph based fragment descriptors : applications to QSAR and beyond.*

July 2007 ISMB 2007, Vienna, Austria. *QSAR: Quantitative Modelling of Molecular Properties and Activities using Chemical Descriptors*.

July 2007 Sanofi-Aventis, Frankfurt, Germany. *Cheminformatics Workflow for Bioactivity and Property Prediction of Chemical Libraries*

July 2007 AIMECS 2007, Istanbul, Turkey. *Predictive QSAR Modeling Workflow and its Application to Support the Experimental Discovery of Biologically Active Compounds*

May 2007 MipTec 2007, Basel, Switzerland. *Cheminformatics approaches to virtual screening*

May 2007 ETH, Zurich, Switzerland. Predictive QSAR Modeling and Virtual Screening

Apr 2007 Molecular Libraries Screening Centers Network and Exploratory Cheminformatics Research Centers Meeting, Philadelphia, PA. *Carolina Exploratory Center for Cheminformatics Research (CECCR): an Update.*

Mar 2007 National American Chemical Society Meeting, Chicago, IL. *Cheminformatics approaches to ligand docking and scoring*

Mar 2007 Biocomputing Day, University of New Mexico, NM. *Imputation of Biological Activities Based on Predictive QSAR Modeling of Screening Data*

Mar 2007 Sanofi Aventis, Paris, France. *Biological Data Analysis and Prediction*

Mar 2007 Therapeutic applications of Computational Biology and Chemistry (TACBAC 2007), Hinxton, Cambridge, UK. *Can Primary High-Throughput Screening Data Be Analyzed In A Meaningful Way*?

Feb 2007 47th Sanibel Symposium, St. Simons Island, Georgia. *Predictive QSAR Modeling and Virtual Screening.*

Jan 2007 International Conference on Chemoinformatics, Pune, India. *Chemoinformatics as Predictive Science*

Nov 2006 Annual Meeting, American Association of Pharmaceutical Scientists, San Antonio, TX. *The Challenges in Predictive QSPR Modeling*

Oct. 2006 eCheminfo and InnovationWell Community of Practice meeting, Bryn Mawr College, Philadelphia. *The statistical significance vs. mechanistic interpretation of ADME/tox models.*

July 2006 Molecular Libraries Screening Centers Network and Exploratory Cheminformatics Research Centers Meeting, Washington, DC. *Carolina Exploratory Center For Cheminformatics Research (CECCR).*

June 2006 CCG user group meeting, Montreal, Canada. *Mining Biomolecular Databases for Structural Motifs: Application to Virtual Screening*

June 2006 Sanofi Aventis, Strasbourg. *Cheminformatics Approaches To Virtual Screening.*

June 2006 World Pharmecutical Congress, Philadelphia, PA. *Robust Computational Framework for Predictive ADMETox Modeling*

May 2006 Dept. of Pharmacy, University of Innsbruck .*Virtual Screening of Biomolecular Libraries Based on Robust Structure-Function Relationship Models*.

May 2006 Dept. of Chemistry, Univ. of Strasbourg. *Predictive QSAR Modeling and Virtual Screening of Biomolecular Libraries.*

May 2006 Schering Foundation International Workshop on GPCRs , Berlin, Germany. QSAR Modeling of GPCRs

May 2006 Workshop: Chemoinformatics in Europe: Research and Teaching Obernai, France. *Cheminformatics Approaches to Virtual Screening*

Apr. 2006 University of Sheffield, UK. *BioMolecular Data Analysis and Molecular Property Prediction using Cheminformatics Approaches.*

Apr. 2006 Department of Chemistry, ULP-Strasbourg. *Quizzing QSAR Models: Truth or Dare?*

Mar. 2006 OpenEye CUPVII annual meeting, Santa Fe, NM. *Carolina Exploratory Center for Cheminformatics Research: Development, Implementation, and Use of the ChemBench system in support of NIH's Molecular Library Initiative*.

Mar. 2006 Pfizer, Groton, CT. *Cheminformatics Approaches To Virtual Screening*.

Dec. 2005 NIEHS Workshop on Virtual Screening, Washington, DC. *Virtual screening of environmental compounds based on chemoinformatics analysis of experimental hts results: Getting Chemistry and Chemoinformatics into the Picture*

Dec. 2005 UNC-Greensboro, Greensboro, NC. *Biomolecular Structure-Function Relationships: Data Modeling, Interpretation, and Virtual Screening of Biomolecular Libraries.*

Nov. 2005 Virginia Commonwealth University, Richmond, VA. *Biomolecular informatics: Identification of Structural Motifs for Functional Annotation of Biomolecules*.

Sep. 2005 University of Lexington, KY. *Chemoinformatics Approaches To Virtual Screening*

July, 2005 Advances in Drug Discovery, Moscow, Russia. *The Unbearable Lightness of In Silico Drug Discovery*

May, 2005 Berlex Biosciences, Richmond, CA. *Chemoinformatic Approaches to Virtual Screening*

April 2005 North Carolina Central University, Cheminformatics Conference, Durham, NC. *The Workflow for Predictive QSAR Modeling*

April 2005 UK QSAR and Cheminformatics Spring Meeting, The University of Surrey, UK. *Quizzing QSAR Models: Truth or Dare?*

Jan., 2005 CHI, Predictive ADME conference, San Diego, CA. *The Workflow for Predictive QSAR Modeling: Model Quality Assessment and Applications to Virtual Screening*

Aug 2004 Sphinx, a Division of Eli Lilly. RTP, NC. *Computer-Aided Discovery and Experimental Validation of Novel Anticonvulsant Agents*

Aug. 2004 ACS, Natl. Meeting, Philadelphia, PA. *Ligand-Based and Structure-Based Approaches to Virtual Screening for Drug Discovery*

Sep. 2004 Schering, Berlin, Germany. *Achieving Real Hits Using Virtual Screening*

Sep. 2004 12th European Conference on QSAR. Ankara, Turkey. *Predictive QSAR Modeling Workflow and its Application to Drug Discovery.*

October 2004 Southeastern Regional Meeting of the American Chemical Society (SERMACS), RTP, NC. *Ligand-Based and Structure-Based Approaches to Virtual Screening for Drug Discover.y*

2003 Duke University, Durham, N.C. "*Computational Geometry of Proteins: From Structure to Sequence to Function"*

2003 E.I. Dupont and Co., Wilmington, DE. "*Validated QSAR Modeling"*

2003 Brystol Myers Squibb, Princeton, NJ. "*The Importance of Being Earnest: Theory and Practice of Predictive QSAR Modeling"*

2003 Inspire Pharmacetical Inc., RTP, NC. "*Predictive QSAR Modeling"*

2003 Trimeris, Inc., RTP, NC. "*QSAR Modeling and Drug Design."*

2003 Mid-Atlantic Regional Meeting of the American Chemical Society, Princeton, NJ. *"Development of Predictive QSPR Models with Application to Database Mining."*

2003 Protein Data Bank, Rutgers University, Piscataway, NJ. *"Computational Geometry of Proteins and Protein/Ligand Complexes."*

2002 Workshop on Computational Protein Structure Analysis, Durham, NC. "*Four-body*

Statistical Potential for Protein Fold Recognition."

2002 Accelrys, Inc., San Diego, CA. *"Structure-Based Drug Design: Scoring Ligand Binding with and without Docking."*

2002 SAR and QSAR in Environmental Research, Ottawa, CA. "*Validated QSAR Models as Virtual Screening Tools*."

2002 Society for Biomolecular Screening, Durham, NC. "*Predictive Datamining Approaches in Chemo- and Bioinformatics*."

2002 224th National Meeting of the American Chemical Society, Boston, MA. "*Application of Chemometric and QSAR Approaches to Scoring Ligand Receptor Binding Affinity."*

2002 224th National Meeting of the American Chemical Society, Boston, MA. "*Evaluation of Ligand-Receptor Binding Affinity with a Novel Statistical Scoring Function Based on Delaunay Tessellation of Protein-Ligand Interface."*

2002 224th National Meeting of the American Chemical Society, Boston, MA. "*Theory and Practice of Safe QSAR."*

2002 North Carolina State University, Raleigh, NC. **"***Computational Geometry of Proteins."*

2002 Pfizer, Inc. Ann Arbor, MI. **"***Computational Geometry of Proteins and Protein-Ligand Complexes"*

2002 Neurogen, Inc, Branford, CT. "*Novel Methods for Predictive QSAR Modeling*."

2001 Chemo/BioInformatics Conference, IBC, San Diego, CA. *"Rational Drug Discovery at the Interface between Chemo and Bioinformatics"*

2001 Duke-UNC Training Program in Medical Informatics. *"Integration of Bio- and Chemoinformatics for Rational Drug Discovery: Do Not Divide...and Conquer."*

2001 COR technologies, Inc., San Fancisco, CA. *"Recent Trends in Computer-Aided Drug Discovery - Benefits and Pitfalls."*

2001 South-East Regional Meeting on Developmental Biology, Ashville, NC. *"Computational Geometry of Proteins: From Structure to Sequence to Function."*

2001 Eighth Annual HTT EXPO: Advancing Drug Development, Philadelphia, PA. *"Biomolecular Informatics: Integration of Bio- and Chemoinformatics Approaches for Drug Discovery"*

2001 Brandeis University. *"Computational Geometry (Delaunay Tessellation) of Proteins: From Structure to Sequence to Function"*

2001 Millenium Pharmaceuticals. *"Variable Selection QSAR."*

2001 Beyond Genomics, Inc, Boston MA. *"From Structure to Function: Structure Based Approaches to Datamining in Chemo- and Bioinformatics."*

2000 Network Science Conference, Charleston, SC. "*Application of Variable Selection QSAR to Database Mining and Combinatorial Library Design.*"

2000 Nankai University, Tianjin, China. *"The Development and Comparative Analysis of Variable Selection QSAR Methods".*

2000 Nankai University, Tianjin, China. *"Variable Selection QSAR Methods and Their Application in Combinatorial Library Design and Database Mining."*

2000 Department of Computer Science, UNC-Chapel Hill. *"Applications of Computational Geometry to Protein Structure Analysis and Drug Design."*

2000 Department of Mathematics, Stanford University. *"Applications of Computational Geometry to Protein Structure Analysis and Drug Design."*

2000 Ortho-McNail Pharmaceuticals, Inc., Raritan, NJ. *"Current Issues in Rational Drug Discovery."*

2000 Moldyn Inc., Boston, MA. "*Correlations vs. Simulations in Drug Design*".

2000 Millenium Pharmaceuticals Inc, Cambridge, MA. "*Rational Drug Design at the Interface between Chemical and Bioinformatics."*

2000 FMC Corporation, Princeton, NJ. *"Recent Developments in Ligand-Based and Structure-*

Based Drug Design Methods."

2000 The Clinical Research Curriculum, UNC-Chapel Hill. *"Computer-Aided Drug Discovery and Design: Methods and Applications".*

2000 The 6th International Symposium on Pharmaceutical Sciences, Ankara, Turkey. "*Applications of Variable Selection QSAR in Drug Design and Discovery."*

2000 First SIAM Conference on Computational Science and Engineering., Washington, DC.. "*Computational Geometry of Molecular Structure"*

2000 QSARs in Environmental Sciences: Crossroads to the XXI Century: Ninth International Workshop on Quantitative Structure Activity Relationships in Environmental Sciences, Burgas, Bulgaria. "*Variable Selection QSAR using 2D Descriptors of Molecular Structures"*

2000 Lions Bioisciences, Inc., Boston, MA. "*Identification of Sequence-Specific Tertiary Packing Motifs in Protein Structures using Computational Geometry."*

1999 Johnson & Johnson Research Corporation. '*Biomolecular Similarity and Diversity in the context of QSAR and Library Design*'

1999 NC Regional Meeting of the National Academy of Sciences, NCSC, Raleigh, NC. '*From Genes to Drugs: A New Stage in Rational Drug Design*.'

1999 217th Meeting of the American Chemical Society, Anaheim, CA. 1. "*Combined Application Of QSAR and Database Mining in Search of Environmental Estrogens*." 2. "*Quick and Dirty? No, Fast And Accurate: The K Nearest-Neighbor QSAR Method*." 3. "*Diversity Sampling: Selection, Space Coverage, and Visualization*."

1999 Tripos, Inc. Symposium on Advances in Drug Design. Duke Inn, Durham, NC. *"Stochastic Sampling of Molecular Diversity: Hit Rates vs. Representation and Coverage of the Diversity Space."*

1999 Department of Computer Science, Ben Gurion University, Beer Sheva, Israel. *"Mathematical Problems in Molecular Modeling: From Drug Design To Protein Structure Prediction."*

1999 Department of Pharmaceutical Chemistry, UCSF School of Pharmacy. "*Correlations vs. Simulations: Choosing the appropriate tool."*

1999 SRC / NASA Ames Workshop on "Self-assembly for Nanoelectronics" NASA Ames Research Center, Moffett Field, CA. *"Correlations vs. Simulations Strategies in Theoretical Analysis of Molecular Recognition."*

1998 Third Pacific Conference on Biocomputing, Maui, Hawaii. '*FOCUS-2D. A New Approach to the Design of Targeted Combinatorial Chemical Libraries.'*

1998 Millenium Pharmaceuticals, Inc., Boston MA. *Rational Approaches to "Irrational" Drug Design: Combinatorial Chemistry and Beyond.'*

1998 Department of Chemistry, University of North Carolina at Wilmington, Wilmington, NC. '*QSAR: Methods and Applications.'*

1998 Airforce Research Laboratory, Dayton, Ohio. The International Workshop on Computational Methods in Toxicology. '*The Development and Comparative Analysis of Variable Selection QSAR Methods.'*

1998 8th International Workshop on Quantitative Structure~Activity Relationships (QSARs) in the Environmental Sciences, Baltimore, MD. 1. '*The UNC QSAR Web Serve*r.' 2. '*The Application of Novel QSAR Models to Screening for Potential Estrogens in Chemical Databases.' 3. 'The Development and Comparative Analysis of Novel Variable Selection QSAR Methods.'*

1998 Rohm and Haas Research Laboratories, Spring House, PA. *"Theoretical Analysis of Chemical Diversity"*.

1998 FMC Research Corporation. '*Computational Analysis of Molecular Diversity and Similarity: From Structure to Function.*'

1998 University of Southern California, Department of Chemistry. '*Computational Approaches*

to Chemical Similarity and Diversity.‘

1998 MSI Workshop on QSAR. ‘*QSAR Methods and Applications*‘

1998 New York University, Department of Chemistry. ‘*Theoretical Approaches to Molecular Similarity and Diversity: From QSAR to Combinatorial Chemistry*.‘

1997 Second Pacific Conference on Biocomputing, Big Island, Hawaii. *“A New Approach to Protein Fold Recognition Based on Delaunay Tessellation of Protein Structure”*.

1997 Second International Symposium on Algorithms for Macromolecular Modelling, Berlin, Germany, May. *Novel Methods for Protein Structure Analysis and Prediction Based on Delaunay Tessellation.*

1997 Gordon Research Conference on QSAR, Tilton, NH, August 1997. *“Unity in Diversity: From QSAR to Combinatorial Chemistry”*.

1997 International congress of quantum chemistry, Savannah, Georgia. “*Theoretical Analysis of Molecular Diversity: Applications to Drug Design.”*

1997 Chemistry Department, University of Georgia at Athens, Athens, GA. “*Rational Design of Combinatorial Chemical Libraries.*“

1997 Vertex Pharmaceuticals, Boston, MA. “*New Computational Methods for Rational Library Design and QSAR*“.

1997 ICAgen, Inc., Research Triangle Park, NC. “*Rational Design of Combinatorial Libraries*.“

1997 University of Illinois, Urbana-Champaigne. “*Statistical Geometry of Protein Structure*.“

1997 Fifth Chemical Congress of North America, Cancun, Mexico. “*Integration of formal training and research in molecular modeling curriculum.***“**

1997 ETH, Zurich, Switzerland. **“***Statistical Geometry of Protein Structure: A New Approach to Structure Analysis and Prediction.***“**

1997 ETH, Zurich, Switzerland. “*Theoretical Analysis of Chemical Diversity in the Context of Combinatorial Chemistry and Drug Design.”*

1997 Department of Chemistry, University of Paderborn, Germany. “*New Tricks for an Old Dog. Novel QSAR Methods and Their Application to Combinatorial Library Design and Database Mining.”*

1997 European Molecular Biology Laboratory, Heidelberg, Germany. ‘*Statistical Geometry of Protein Structure: A new Approach to Structure Analysis and Prediction.’*

1996 First Pacific Conference on Biocomputing, Big Island, Hawaii. *“Statistical Geometry Analysis of Proteins: Implications for Inverted Structure Prediction”*.

1996 National Cancer Institute, NIH, Frederick, MD. *“Statistical Geometry of Protein Structure”.*

1996 Chemistry Department, University of Georgia at Athens, Athens, GA.*“New Computational Approaches to QSAR and Combinatorial Chemistry”.*

1996 Chemistry Department, University of Georgia at Athens, Athens, GA.*“A new Approach to Protein Fold Recognition Based on Delaunay Tessellation of Protein Structure”.*

1996 Chemistry Department, UNC-Chapel Hill. *“Statistical Geometry of Protein Structure: A new Approach to Protein Fold Recognition”*.

1996 Mid-Atlantic Pharmacology Society 1996 Fall Meeting, Raritan, New Jersey. *“New Dimensions in Drug Design: From QSAR to Combinatorial Chemistry”*.

1996 Rohm and Haas Research Laboratories, Spring House, PA. *“Theoretical Analysis of Chemical Diversity in the Context of Drug Design”*.

1996 Southeast Regional Meeting of the American Chemical Society Greenville, South Carolina. *“The Combined Application of 2D QSAR and Computational Combinatorial Chemistry Approaches to De Novo Ligand Design”*.

1996 Guest of Honor at The Meeting of the Computational Chemistry Section of the German Chemical Society, Paderborn, Germany. “*Unity in Diversity*”.

1996 The Workshop on the Protein Folding Problem: Analysis and Prediction of Protein Structure. Chapel Hill, NC. *“A Statistical Geometry Approach to Protein Structure*

Analysis and Prediction".

1995 Molecular Dynamics User Group, North Carolina Supercomputing Center, RTP, North Carolina. *"Free Energy of Folding and Refolding of Model Dipeptides in Aqueous Solution"*.

1995 The Scripps Research Institute, La Jolla, CA. *"Relative Free Energies of Folding and Refolding of Model Dipeptides in Aqueous Solution"*.

1995 The Pembroke University, Pembroke, N.C. *"Recent Developments in Three-Dimensional QSAR: Applications to Molecular Modeling of Inhibitors of Acetylcholinesterase"*.

1995 Chemistry Department, University of Georgia at Athens, Athens, GA. *"Recent Surprises and New Developments in 3D QSAR".*

1995 Division of Pharmaceutics, School of Pharmacy, UNC-CH. *"Computer-Assisted Drug Design".*

1995 Department of Biochemistry, North Carolina State University. *"Statistical Geometry Analysis of Folded Proteins: Implications for Inverted Structure Predictions".*

1995 Medical College of Virginia, Richmond, VA. *"A QSAR Journey: From 2D QSAR to 3D QSAR and Back".*

1995 Medical College of Virginia, Richmond, VA. *"Statistical Geometry Analysis of Proteins"*.

1994 University of Georgia, Athens, GA. *"Relative Free Energy of Folding and Refolding of Model Dipeptides in Aqueous Solution."*

1994 Molecular Simulations, Inc., Boston, MA. *"Modern Methods in Rational Drug Design."*

1994 XIII International Symposium on Chemical Education, San Juan, Puerto-Rico. *"Molecular Dynamics Simulations"*.

1994 XXX Congress of the Sociedad Quimica de Mexico, Cancun, Mexico. *"Molecular Modeling of Acetylcholinesterase Inhibitors: an Example of Integrating Teaching and Research"*.

1994 Brain and Development Center Seminar Series, UNC-CH. *"Application of Molecular Simulations to Problems of Protein and Drug Design"*.

1993 American Peptide Symposium, Alberta, Canada. *"Relative Free Energies of Folding and Refolding of Model Secondary Structure Elements in Aqueous Solution."*

1993 The DuPont Merck Pharmaceutical Company, Wilmington, DE. *"Applications of Molecular Simulations to Protein and Drug Design."*

1993 The National Institutes of Health, Bethesda, MD. *"Relative Free Energy of Folding, Refolding, and Inverted Folding of Model Dipeptides in Aqueous Solution."*

1992 Burroughs Wellcome Co., Research Triangle Park, NC. *"Relative Binding Affinity of HIV-1 Protease Inhibitors to the Protease from Free Energy Simulations."*

1990 SmithKline & French Co., King of Prussia, PA. *"Hydrophobic-Hydrophilic Amino Acid Interactions in Protein-Protein Recognition."*

GRANT HISTORY:

Pending research grants.

1. Drug Repurposing for Cancer Therapy: From Man to Molecules to Man. PI. **NIH**
2. Integrating cheminformatics and molecular simulations for virtual drug screening. coPI; PI: Nikolay Dokholyan. **NIH**.
3. Materials Informatics: Mining, Visualizing, and Designing Materials with the Desired Properties. (PI: Tropsha). **NSF**.
4. SI2-SSI: Collaborative Research: Nanomaterial Registry: an Interactive Research Resource for Promoting Progress in Nanoscience. NSF
5. Materials Informatics Guided Design of New Solar Cell Electrodes. PIs Cahoon and Tropsha, NSF
6. Materials Informatics Platform for Property Prediction. Office of Naval Research.

Currently funded research grants (Principal Investigator).

1. ABI Program: Innovation: Synergistic application of cheminfomatics and computational geometry approaches for modeling protein-protein interactions. **NSF** 10-567 Advances in Biological Informatics. (10%) Total direct (per year) : $200,000. 8/01/12-7/31/16.
2. ChemBench: the Integrated Web Portal to Accelerate Cheminformatics and Chemical Genomics Research. Total direct (per year) : $190,000, **NIH**, R01 GM 096967-01A1. (10%).
3. Materials Informatics: Expansion of the Aflowlib Database of Electronic Properties of Materials and the Development of Novel Materials Fingerprints for Efficient Database Mining and QSPR Modeling. **US Office of Naval Research**, N000141310028 (8%), Total cost $125K/year, dates 01/01/2013-12/31/2016.
4. PhACTS (Physiologically Accurate Community-based Framework for Training Systems). Applied Research Associates, Inc./ Dept. of Defense; Role: Consortium PI. S-001903/ W81WH-13-2-0068 (PI: Heneghan). 9/15/2014 – 12/15/2015, Total Cost. 350K
5. A Virtual Environment to Enhance Education, Practice, and Research in Pharmacy. Eshelman Institute for Innovation, 10/1/2015 – 9/30/2018. Total cost: $1,994,776

Currently funded research grants (Co-Investigator).

6. Carolina Center For Computational Toxicology: Experimental and computational tools for NexGen safety assessments. EPA RD83382501 (PI: Rusyn; coPI: Tropsha). 9/1/2011 – 8/30/2015. Total Cost: 1.2M (Tropsha lab: 60K/year direct).
7. NC TraCS. delAQUA – Computer-Assisted Drug Solubilization Platform (4DR11404; 50K); PI: Sasha Kabanov.
8. Nano Approaches to Modulate Host Cell Response for Cancer Therapy; Project 4 title: High Capacity Polymeric Micelle Therapeutics for Lung Cancer. NIH/NCI; Role: Project 4 Investigator; Project 4 Direct Costs: $343,636

Completed projects.

9. Computer-Aided Design of Nanomaterials with the Desired Bioactivity and Safety Profiles. **Semiconductor Research Corporation**. Y502164 (3%). Total cost: 125,600/year for three years. 1/1/2012 – 12/31/2014
10. Predictive QSAR models of hepatotoxicity. **EPA RD 83499901** (10%).Total Direct Cost: 500K Dates: 5/1/2011 – 4/30/2014.
11. Disposition of Flavonoids via Metabolic Interplay. NIH NOT-GM-08-130. 08/01/10-07/31/13. Direct cost to Tropsha lab: $39,930 (per year),
12. Bioengineering Partnership to Improve Chemical Hazard Testing Paradigms (Rusyn). NIH ES015241. Dates 12/1/2007 – 11/30/2012; co-PI (10%). Total cost $2,478,676 (ca. 125K direct to Tropsha Lab)
13. Carolina Center for Computational Toxicology (Rusyn), EPA RD 83382501. Dates: 4/1/2008 – 3/31/2012; co-PI (10%). Total cost $3.2M (ca. 120K direct per year to Tropsha lab)
14. Computational Models and High-Throughput Cellular-Based Toxicity Assays for Predictive Nanotoxicology (5%; R. Mumper coPI). Funding source: Semiconductor Research Corporation. Dates: 3/1/2009 – 2/29/2012(300K total for 3 years).
15. Predictive QSAR Modeling (ARRA Competitive Supplement). **NIH R01GM066940-06S** (10%). Dates 9/30/2009 – 8/31/2011. Total direct cost 500K; First year cost 250K.
16. Regulation of androgen receptor by HER-2 and Ack1 tyrosine kinases. (coPI 0%; Whang, YE - PI). **NIH 3R01CA120921-02S1** (ARRA Supplement). Dates: 08/01/2009 – 07/31/2011. Total cost: $396,640; first year direct cost $134K (ca. 80K to Tropsha lab)
17. Carolina Environmental Bioinformatics Research Center (Wright). **EPA RD832720**. Dates: 9/1/05 – 8/31/11. Section PI (10%). Total cost: $4,500,000 (ca. $725,000 direct to Tropsha lab).
18. Robust Computational Framework for Predictive ADMETox Modeling (15%). **NIH R21GM076059.** Dates: 6/1/06 – 5/31/11. Total direct cost $732,375.
19. Protein Structure/Function Specific Packing Motifs (10%). **NIH**. Dates: 8/1/06-7/30/11. Total direct cost - $760,000.

20. Disposition of Flavonoids via Metabolic Interplay. NIH R03GM070737 (PI: Ming Hu, UH; Tropsha: subcontract PI). Dates: 8/1/ **GM068665**2010 – 7/31/2011. Total: $179,463.
21. Developing Novel Cheminformatics Tools to Accelerate the Search for Cancer Therapeutics. UCRF (100K total and direct). Dates: 3/1/2009 – 2/28/2011.
22. To develop and deliver to BICL validated QSPR models for human intestinal drug transport. Contract with Boehringer Ingelheim (99.5K). Dates: 3/1/2009 – 2/28/2010
23. Development of Robust Computational Models of Chemical Toxicity for Health and Environmental Risk Assessment (US PI; Afantitis – Cyprus PI). Funding source: Research Promotion Foundation, Cyprus. Dates: (Total 26K).
24. UNC Predoc. Program in Bioinformatics and Computational Biology. **NIH NGA: 1 T32 GM067553-01A1**. First year direct cost $112,118 (NOTE: transferred the PI to Dr. Tim Elston in summer 2006)
25. UNC-CH Research Training Program in Bioinformatics and Computational Biology. Principal Investigator. **UNC-GA**. Dates: 07/01/05– 06/30/08. Total Cost: $250,000. First year direct cost: $50,000. (NOTE: transferred the PI to Dr. Tim Elston in summer 2006)
26. Carolina Exploratory Center for Cheminformatics Research (15%). **NIH P20HG003898**. Dates 9/1/05-8/31/09. Total direct cost: $750,000
27. Carolina Center for Exploratory Genetic Analysis. **NIH P20-RR20751** (Reed). Co-investigator (5%). Dates: 6/1/2004 – 5/31/2006. Total Direct Cost: 750K.
28. Novel Computational Tools to Identify Residue Motifs from Protein Graphs (Wang). NSF 0523875 Co-investigator (5%). Dates: 10/1/05 – 9/30/08.
29. Systematic Discovery of Automatic Gene Regulation Modules in Cell Cycle Dynamics (4%). Elsa A. Pardee Foundation, total first year direct cost $54,000
30. Computational Geometry for Structural Biology and Bioinformatics (Edelsbrunner). Co-PI (5%). **NSF CCR-0086013**.
31. ANCA Glomerulonephritis: From Molecules to Man. **NIH 1PO1 DK58335-01**. Co-Investigator, 18% salary support (R. Falk, P.I.). Total direct cost $3,749,939; 1st year direct cost $749,950. Dates: 7/1/2000 – 6/30/05.
32. UNC-CH Research Training Program in Bioinformatics and Computational Biology. Principal Investigator (10% effort). **UNC-GA**. Dates: 07/01/02 – 06/30/05. Total Cost: $450,000. First year direct cost: $150,000.
33. Predictive QSAR Modeling (Minority Supplement) – PI. **NIH. R01GM066940-01A1S1**. $26,842 direct cost. Dates: 8/15/03-8/14/04.
34. Testing Hypothesis about Proteins using High Throughput Methods. Co-Investigator, 5% salary support and $15,000 equipment (PI: M. Edgell, Department of Microbiology & Immunology, UNC-CH). North Carolina Biotechnology Multi-Disciplinary Research Program, **North Carolina Biotechnology Center**. Project Period: 02/01/2002-2004. $200,000 direct costs per year.
35. Duke-UNC Training Program in Medical Informatics. National Library of Medicine, **NIH/NLM** LM07071 (20%). Dates: 07/01/01 – 06/30/02 (no cost extension until 6/30/2004). Total Cost: $756,654.
36. Bioinformatics Research Training Supplement to Duke-UNC Training Program in Medical Informatics: (5%). **NIH/NLM**. Dates. 7/01/01 – 6/30/02 (no cost extension until 6/30/03). Total Cost: $194,127.
37. Health Informatics Supplement to Duke-UNC Training Program in Medical Informatics: (3%). **NIH/NLM**. Dates. 7/01/01 – 6/30/02 (no cost extension until 6/30/03). Total direct cost: $50,000.
38. Computational Analysis of Proteins: From Structure to Sequence to Function. **NSF MCB-0112896** (10%). Dates: 10/01/01 – 09/30/04. Total cost: $301, 619.
39. Protein Structure and Function Prediction for Genomic Sequences: The Next Step in the Genomic Revolution, NCI 1999032. North Carolina – Israel Research Partnership (10%; Principal Investigator, Israel – Prof. D. Fischer). **NCI**-SRP # 1999032; 2/01/01 – 1/31/03. Total direct cost: $218,00, current year direct cost: $71,129.

40. Design of Novel D1 Dopamine Receptor Ligands (PI; 10% salary). **NIH** R03 MH60328-01, 7/1/00-6/30/02 (no cost extension until 6/30/03). Annual direct cost $49,699.
41. NIH Biomedical Research Technology Program. "Parallel Computing Resource for Structural Biology" (Co-Principal Investigator, 15% of effort, Principal Investigator - J. Hermans) R01 RR08102. 10/01/98-09/30/03. $605,903.
42. FLEX-DOCK: Flexible Docking Using Modal Methods (Subcontract PI of the SBIR Proposal, NIH; 10% effort). NIH RR10687-02A1. 7/1/98-6/30/00, Annual direct cost of the subcontract $61,984.
43. Novel Molecular Site for Antidopaminergic Action. Source of funding: NIH, # MH 40537 (co-investigator, 20% efforts; P.I. Professor R. Mailman). Dates: August 1, 1992 - May 31, 1997. Annual Direct cost - $197.099.
44. Major Expansion of Computer Facilities for Scientific Research (Co-Principal Investigator; Principal Investigator Professor J. Hermans). Dates: 08/01/1993 - 01/31/1996, $76,328 annual direct cost. Source of funding: National Science Foundation, BIR-9123574, Biological Instrumentation Program.
45. NIH Biomedical Research Technology Program. "Parallel Computing Resource for Structural Biology" (Co-investigator, 15% of effort, Principal Investigator - J. Hermans), 12/01/92-11/31/97, $2,391,704 total direct cost.
46. Hoechst-Roussel Pharmaceuticals Inc. "Basic Research in Dopamine Neurotransmission" Richard Mailman, P.I.; Alexander Tropsha, Section P.I.: (5% effort) Dates 1/1/95-12/31/96, current year budget (direct costs): $377,000 total, $78,483 Tropsha project.
47. Hoechst Celanese Corporation/UNC-CH Research Partnership. Molecular Simulations of β-amiloid peptides. Dates: July 1, 1995-June 30 1996. Amount Funded: $25,000.
48. A_Novel Method for Protein Structure Prediction from Sequence. Source of funding: School of Pharmacy Faculty Seed Grant Program. Dates: January 1996 - December 1996. Amount funded: $4,000 direct cost.
49. Hoechst Celanese Corporation/UNC-CH Research Partnership Computer-Aided Molecular Modeling and Rational Design of Acetylcholinesterase Inhibitors. Dates: July 1, 1994-June 30 1995. Amount Funded: $25,000.
50. Application of Free Energy Simulations to the Binding of the Transition-State-Analog Inhibitor to HIV Protease (Principal Investigator, 80% of effort). Source of funding: North Carolina Supercomputing Center. Dates: July 1, 1991 - June 30, 1992. Amount funded: 200 hours of Cray Y-MP time.
51. Molecular Dynamics Studies of the Stability of Coiled Coils (Principal Investigator, 20% of effort). Source of funding: Cray Research Inc. and North Carolina Supercomputing Center. Dates: January 1992 - December 1992. Annual Direct Cost - $7,000 and 90 hours of Cray Y-MP time.
52. The Application of Molecular Dynamics and Free Energy Simulations to Protein Engineering: Computer-assisted Rational Design of Betabellins and Coiled Coils (Principal Investigator, 20% of effort). Source of funding: Cray Research Inc. and North Carolina Supercomputing Center. Dates: January 1993 - December 1993. Annual Direct Cost - $7,000 and 180 hours of Cray Y-MP time.
53. Free Energy Analysis of Beta Turns (Principal Investigator - 20% of effort). Source of funding: North Carolina Supercomputing Center. Dates: February 28, 1992 - February 28, 1993. Amount funded: 260 hours of Cray Y-MP time.
54. Molecular Modeling of HIV Protease Inhibitors (Principal Investigator, 10% of efforts). Source of funding: School of Pharmacy Faculty Seed Grant Program. Dates: June 1993 - May 1994. Amount funded: $5,300 direct cost.
55. Theoretical Studies of the Preferred Pairwise Amino Acid Interactions (Principal Investigator, 100% of effort). Source of funding: The University of North Carolina Research Council Research Grant. Dates: 3/3/92-10/1/93. Amount funded: $3,000 direct cost.
56. Computer Simulations of the Role of Hydrophobic-Hydrophilic Amino Acid Interactions in Proteins. UNC-CH Junior Faculty Development Award. Principal Investigator, 100% of effort. Dates: 01/01/1993 - 12/31/1993, $3,000.00 total direct cost.

57. UNC/IBM Joint Study Agreement (Principal Investigator, 50 % of effort). Source of Funding: The University of North Carolina and IBM Co. Dates: 5/1/1992-4/30/1993. Amount funded: $63,000 provided by UNC, and donation of the computer equipment by IBM in the amount of $51,826.00
58. North Carolina Symposium on Molecular Modeling (Principal Investigator). Source of Funding: North Carolina Biotechnology Center. Amount Funded: $2,000.00

INDUSTRIAL FUNDING

Unrestricted Research Support, Glaxo Research Institute, 1992 ($50,000)
Unrestricted Research Support, Macronex, Inc. 1993 ($15,000)
Unrestricted Research Support, Rohm & Haas, 1997-1998 ($30,000)
Unrestricted Research Support, Rohm & Haas, 1998-1999 ($30,000)
Unrestricted Research Support, FMC Corporation, 1999 ($20,000).
Unrestricted Research Support, Glaxo Wellcome, 2000 ($18,000)
Unrestricted Research Support, Glaxo Wellcome, 2001-2002 ($18,000)
Unrestricted Research Support, Scynexis, Inc., 2001 ($12,000)
Software Licensing Fees: Millennium Pharmaceuticals, Inc., 2001 ($40,000)
Software Licensing Fees: Ortho-McNail Pharmaceuticals., 2001 ($30,000)
Contract Research: COR Pharmaceuticals, 2002 ($7,000).
Unrestricted Research Support, GlaxoSmithKline, 2002 ($37,000)
Unrestricted Research Support, Eli Lilly, 2002 ($15,000)
Unrestricted Research Support, Syngenta, 2002 ($30,000)
Unrestricted Research Support, Pfizer,Inc, 2002 ($20,000)
Unrestricted Research Support, Eli Lilly, 2003 ($15,000)
Unrestricted Research Support, Inspire Pharmaceuticals, 2002 ($25,000)
Unrestricted Research Support, Pfizer,Inc, 2003 ($30,000)
Unrestricted Research Support, Eli Lilly, 2004 ($30,000)
Unrestricted Research Support, Berlex Biosciences, 2004 ($5,000)
Contract Research Support, Berlex Biosciences, 2005 ($80,000)
Contract Research Suppport, Sanofi-Aventis, 2006 ($50,000).
Contract Research Support, Boehringer Ingelheim, 2009-2011 ($97K)

TEACHING

1991-present: Instructor, Introduction to Molecular Modeling and Computer-Assisted Drug Design (MEDC805). This course (required for MedChem students) introduces basic principles of molecular modeling techniques, with the emphasis on drug design. Two-three lectures a week plus three-four hour hands-on laboratory practice. The course is taught every fall. Typical enrollment 5-6 students.

1991-2007: Instructor, Introduction to Macromolecular Modeling (MEDC804/BIOC804). This course introduces principles of protein structure organization and classification, molecular simulations of proteins, and structure based drug design approaches. Two-three lectures a week plus three-four hour hands-on laboratory practice. The course is taught every spring. Typical enrollment 10-12 students.

CONTINUING EDUCATION:

1991-2010: Instructor, the American Chemical Society Short Course on Molecular Modeling. The course is being taught twice a year at the University of Georgia, Athens, Georgia

(1991-1997), UT Austin (1997-2005), UNC-Greensboro (2006) and once or twice a year in conjunction with the National Meetings of the American Chemical Society..

1993: Organizer and instructor, two three-day workshops on molecular modeling for scientists from Hoechst Celanese Corporation and Hoechst-Roussel Pharmaceuticals, Inc. The workshops were given within the framework of the UNC/HCC partnership.

1995: Instructor, Introductory Molecular Modeling Workshop, North Carolina Supercomputing Center.

1995 Organizer and Instructor for Carolina Workshop on Computational Molecular Biology.

1996 Organizer and Instructor, five day Introductory Workshop on Molecular Modeling And Drug Design, Caracas, Venezuela.

1996 Organizer and Instructor, five day Introductory Workshop on Molecular Modeling And Computational Chemistry, Mexico-City, Mexico.

1996 Organizer and Instructor, Carolina Workshop on Computational Molecular Biology, UNC-Chapel Hill.

1999 Instructor, a three day Introductory Workshop on Molecular Modeling and Drug Design, FMC Corporation, Princeton, NJ, Feb. 1999.

RESEARCH GUIDANCE

The following is a list of individuals who have conducted/are conducting research under my immediate supervision.

A. Research Associates:

Former:

-Dr. I. Vaisman, Research Assistant Professor, Oct. 1992-2000 (Present position: Associate Professor, George Mason University, Manassas, VA).

-Ms. K. Krishnaswami, Research Associate (jointly with Prof. P. Smith, Division of Pharmaceutics, School of Pharmacy), April 1993-April 1994.

-Dr. Thomas O'Connell, Research Assistant Professor, Oct. 1994 – June 1997 (present position: Director of Metabolomics Core, UNC-CH).

-Dr. Adriana Vidal, Postdoctoral Research Associate, September 1994 – 1995 (present position: Research Associate, Duke University).

-Dr. Sun Jin Cho, Postdoctoral Fellow, September 1995 – 1997 (present position: Research Scientist, Amgen).

-Dr. Ganesh S. Ethiraj, Postdoctoral Fellow, Sep. 1997 – March 1999 (present position: Research Scientist, Chemical Abstract Service, Columbus, Ohio)

- Dr.. YunDe Xiao, Postdoctoral Fellow, 1999- 2001 (present position: Research Scientist, Targacept, Inc., Winston-Salem)

- Dr. Patricia de Cerqueira Lima, Postdoctoral Fellow, 2002 –2003.

- Dr. John Grier, NLM Postdoctoral Trainee, 2001 – 2004.

- Dr. Peter Itskowitz, Postdoctoral Fellow, 2003-2005

- Dr. Weifan Zheng, Research Associate Professor, 2004 – 2006 (present position: Associate Professor, NCCU)

- Dr. Lin Ye, Postdoctoral Fellow, 2007-2009 (present position: Research Scientist, FDA)

- Dr. Georgiy Abramochkin, Postdoctoral Fellow, 2007 – 2009

- Dr. M. Karthikeyan, Res. Asst. Prof., 2007-2009.

- Dr. Simon Wang, Research Assistant Professor, 2005 – 2010 (Current position; Assistant Professor, Howard University, Washington, DC)

- Dr. Hao Zhu, Research Assistant Professor, 2006 - to–2010. Current Position: Assistant Professor, Rutgers University at Camden, NJ

- Dr. Aleks Sedykh, Postdoctoral Fellow, 2008 – 2013. Current Position: Research Scientist, MultiCASE, Cleveland, OH.

- Dr. Nancy Baker, Postdoctoral Fellow, 5/2010 – 10/2011.Curent Position Research Scientist, EPA.
Dr. Denis Fourches, Postdoctoral Fellow, 2008 – 2/2010; Res. Asst. Prof. from 3/2010 – 12/2014. Current position: Asst. Prof. Department of Chemistry, NCSU

Current:

- Dr. Alexander Golbraikh, Research Associate Professor, 1999 - to–date.
- Dr. Clark Jeffries, Research Professor, 2005 – to-date.
- Dr. Eugene Muratov, Postdoctoral Fellow, 2009 – 2011; Res. Prof from 2011.
-Dr. Olexander Isayev, Research Scientist, 2013 – present.

B. Graduate Students (Major Advisor)

Former:

Weifan Zheng	Ph.D., Medicinal Chemistry, 1997. Thesis: *"Novel Computational Techniques for Rational Drug Design: Combinatorial Library Design, Database Mining, and QSAR Analysis"*. (Present position: Associate Professor, NCCU).
Xin Chen	Ph.D., Medicinal Chemistry, 1998. Thesis: *"Novel Computational Methods for Drug Discovery and Design: Recursive Partitioning of Pharmaceutical Databases, Automated Pharmacophore Identification, and Fast Free Energy Calculations."* (Present position: Research Scientist, Ortho-McNail Pharmaceutical).
Stephen Cammer	Ph.D., Medicinal Chemistry, 2000. Thesis: *"Computational Geometry of Protein Structure: Analysis, Comparison, and Annotation."* (Present Position: Assistant Professor, VBI, Blacksburg, VA).
Yuanyuan Qiao	Ph.D., Chemistry (Nankai University, China), 2003. Present position: Associate Professor, Nankai University, China.
Jun Feng	Ph.D., Medicinal Chemistry, 2002. Thesis: *"Efficient Computational Tools for Structure Based Drug Design."* (Present position: Vertex Pharmaceuticals, Cambridge, MA).
Min Shen	Ph.D., Medicinal Chemistry, 2004. Thesis: *Implementation and Application of Machine Learning Algorithms in Computer-Assisted Drug Design.* Present Position: Research scientist, Lexicon Pharmaceuticals, Princeton, NJ.
Bala Krishnamoorthy	Ph.D., Operations Research, 2004. Present position: Assistant Professor, Department of Mathematics, Washington State University, Pullman WA
Crystal Wright	M.S., Biomedical Engineering, 2004.
Scott Oloff	Ph.D., Pharmacology, 2005. Thesis: *Development of computer aided drug discovery methods based on machine learning techniques and application to the dopamine D1 receptor*. Present Position: Research scientist, Boehringer Ingelheim, Ridgefield, CT.
Shuxing (King) Zhang	Ph.D., Medicinal Chemistry, 2005. Thesis: *Development and Application of Novel Computational Approaches for Computer-Assisted Drug Design (CADD) and Protein Modeling* . Present position: Asst. Prof., The University of Texas M. D. Anderson Cancer Center, Houston, TX.
Shuquan Zong	PhD., Biomedical Engineering, 2005. Thesis: *Application of statistical geometry to protein folding*. Present Position: Research specialist, UNC-CH.
Ruchir Shah	Ph.D., Material Sciences, 2006. Thesis: *Computational analysis of protein function and protein-protein interactions* . Present position: Research Scientist, Constella Research, RTP, NC
Raed Khashan	PhD., Medicinal Chemistry, 2007. Thesis: *Development and application of ligand-based and structure based computational drug discovery tools based on frequent subgraph mining of chemical structures*

Kun Wang	PhD., Medicinal Chemistry, 2009. Thesis: *Classifier Design to Improve Pattern Classification and Knowledge Discovery for Imbalanced Datasets*
Amie Rogers	MS, Environmental Engineering (co-advised with Prof. I. Rusyn), 2010. Thesis: *Quantitative Structure Activity Relationship (QSAR) Modeling Of Human Liver Adverse Effects Database Using K-Nearest Neighbor (kNN) Method*.
Reema Hajou	PhD., Medicinal Chemistry, 2010. *In Silico Strategies to Study Polypharmacology of G-Protein-Coupled Receptors*.
Chris Grulke	PhD., Medicinal Chemistry, 2011. *Development and Extension of Cheminformatics Techniques for Integration of Diverse Data to Enhance Drug Discovery*
Jui-Hua Hsieh	PhD., Medicinal Chemistry, 2011. *Cheminformatics Approaches to Structure Based Virtual Screening: Methodology Development and Applications*
Hao Tang	PhD., Biochemistry & Biophysics, 2011 *Prioritizing Small Molecules for Drug Discovery or Chemical Safety Assessments from Ligand- and Structure-Based Cheminformatics Approaches*
Liying Zhang	PhD., Medicinal Chemistry, 2011. *Development and Application of Cheminformatics Approaches to Facilitate Drug Discovery and Environmental Toxicity Assessment. Current position: Senior Research Associate in Department of Biochemistry HTS/RNAi Screening Core, UT Southwestern Medical Center*
Man Luo	PhD., Medicinal Chemistry, 2011. *Cheminformatics Modeling of Diverse and Disparate Biological Data and the Use of Models to Discover Novel Bioactive Molecules*
Guiyu Zhao	PhD., Medicinal Chemistry, 2011. *The QSARome of the Receptorome: Quantitative Structure-Activity Relationship Modeling of Multiple Ligand Sets Acting at Multiple Receptors*
Tanarat Kietsakorn	MS., Medicinal Chemistry, 2011. *Protein Function Prediction using Family-specific Structural Motifs*
Dongqiuye Pu	MS, Molecular Pharmaceutics, 2012 *Quantitative Structure-Toxicity Relationship Modeling of Organic Compounds and Nanoparticles*
Tony Wu	PhD., Biomedical Engineering, 2012. *Novel Cheminformatics Methods for Modeling Biomolecular Data in High Dimension Low Sample Size (HDLSS) Chemistry Space*
Yen Low	PhD, Environmental Science and Engineering, 2013. *Toxicity Prediction Using Multi-disciplinary Data Integration and Novel Approaches*
Petro Borisov	PhD, Statistics and Operations Research (co-advised with Steve Marron), 2013. Statistical Methods in Chemoinformatics.
Stephen Bush	PhD, Bioinformatics and Computational Biology, 2013. Novel Cheminformatics Approaches for Modeling Protein-Protein Interactions. Current Position: postdoctoral fellow, UT Southwestern.
Andrew Fant	PhD, Medicinal Chemistry, 2015. The effect of data curation on the accuracy of quantitative structure-activity relationship models. Current position: Postdoctoral Fellow, FDA.

Current:

Stephen Capuzzi	PhD, Medicinal Chemistry, 2018 (anticipated)
Sherif Faraq	PhD, Medicinal Chemistry, 2019 (anticipated)

C. Visiting Fellows, rotation, and honors students:

2014: Mary La, PY3, School of Pharmacy
2014: Hugh Heldenbrand, PY1, School of Pharmacy
2014-present. Vinicius Alves, visiting graduate student, Federal University of Goiás, Brazil

Past:

-Prof. J. Bier, Ferrum College, WV, Visiting Scientist. Supported by Burroughs Wellcome Scholarship Fund, 1993-1994 (one year).
-Prof. M.L. Serrano G., Universidad Central De Venezuela, Visiting Scientist, 1993 (four months).
-Prof. Ramiro Araya, Universidad de Santyago, Chile, 1996 (supported by a grant from ACS).
- Michael Morgan, Honors M.D. Program, UNC Chapel Hill, 1993-1994.
- Christian Pilger, Unversity of Paderborn, Germany, 1998
- Axel Dietrich, Unversity of Paderborn, Germany, 1997
- David Bostick (rotation student), Summer 2000 (Ph.D. candidate, Department of Physics, UNC-Chapel Hill)
- Sagar Khare (rotation student), 2002 (Ph.D. candidate, Department of Biochemistry and Biophysics, UNC-Chapel Hill).
- Luke Huan (rotation student), 2002 (Ph.D. candidate, Department of Computer Science, UNC-Chapel Hill).
- Andrew Leaver-Fay (rotation student), 2002 (Ph.D. candidate, Department of Computer Science, UNC-Chapel Hill).
- Assia Kovacheva, University of Vienna, Visiting Scientist, 2002 (three months) and 2003 (four months).
- Berk Zafer, Ankara University, visiting scholar, 2005 (3 months)
- Won-Jea Cho, Prof., College of Pharmacy, Chonnam National University, Korea (2004-2005).
- Dr. Achintya Saha, Visiting Scientist, 2007 – 2008
- Mr. Tiago Moda, Visiting Graduate Student, University of Sao Paolo, Brazil 6/2009 – 5/2010
- Mr. Vinicius Alves (Brazil), 2012
- Mr. Xiangwei Zhu (China), 2012

D. Technical Personnel.

Ian Kim, Research Programmer

MEMBERSHIPS IN PROFESSIONAL SOCIETIES:

1990-present	American Chemical Society.
1991-present	American Association of Colleges of Pharmacy.
1992-present:	American Association for the Advancement of Science.
1993-1998:	Drug Information Association.
1993-1995:	American Protein Society.

UNIVERSITY SERVICE

Administrative Positions:

Associate Dean for Research and Graduate Education, 2011 – present.

Chair, MCNP Division, 2005 – 2011.
Associate Director, Carolina Center for Genome Sciences, 2001 – 2006.
Founding Director, UNC Bioinformatics and Computational Biology Training Program, 2002-2006.
Director, Graduate Studies, Division of Medicinal Chemistry and Natural Products, School of Pharmacy, 2001 – 2002.

Committee memberships

1993-1994:	Search Committee for the Division Chairman
1994-1995:	Division of MCNP Faculty Search Committee
1997-1998:	School of Pharmacy Vanguard Committee
1996-1997:	Chair, Faculty Search Committee
1999:	School of Pharmacy Screening committee for the Associate Dean, Graduate Education and Scholarship
2000 – 2002:	Graduate Education and Research Committee, School of Pharmacy.
2000:	Division of MCNP Faculty Search Committee
2002-2003:	UNC Computational Resource Coordinating Committee for Genomics and Bioinformatics
2011 - present:	ESOP Full professors Committee; Executive Committee; Space Committee; COI Committee (Chair)
2011-present:	Member, UNC Conflict of Interest Committee;
2013 – present:	University Health Informatics Committee
2012-present:	Member, CTSA steering committee

Student Ph.D. Advisory Committees

Y. Yan, Ph.D. Chemistry (co-advisor); graduated 1994.
X. Chen, Ph.D. Medicinal Chemistry; graduated 1994.
J. Rozzelle, Ph.D. Chemistry (co-advisor); graduated 1995.
J. Cho, Ph.D. Medicinal Chemistry; graduated 1995.
V. Watts, Ph.D. Pharmacology; graduated 1996.
D. Hoffman, Ph.D., Computer Science; graduated 1996.
N. Choksi, Ph.D. Medicinal Chemistry; graduated 1998.
B. Hoffman, Ph.D. Medicinal Chemistry; graduated 1998.
C. Owens, Ph.D. Medicinal Chemistry; graduated 1999.
A. Hussain, Ph.D. Medicinal Chemistry; graduated 1999.
K. Chen, Ph.D. Medicinal Chemistry, graduated 1999.
B. Barnes, Ph.D. Medicinal Chemistry; graduated 1999.
C. MacLaughlin, Ph.D. Medicinal Chemistry; graduated 2000.
E. Bucholtz, Ph.D., Medicinal Chemistry; graduated 1998.
D. VanVliett, Ph.D., Medicinal Chemistry; graduated 1998.
Sang Hyup Lee, Ph.D. Medicinal Chemistry; graduated, 2003.
Zhiyan Xiao, Ph.D. Medicinal Chemistry; graduated, 2003.
Jacqueline Legere, Ph.D. Medicinal Chemistry; graduated 2004.
Liza Proctor (graduated 2013)
Brian Der (graduated 2013)
Ardeshir Golalei (Chemistry)

EXTRA-UNIVERSITY SERVICE

Committee memberships

1993-1998. Member: Awards Committee, American Association of Colleges of Pharmacy:

1999 – 2004:	Member, Executive Committee, Division of Computers in Chemistry, ACS:
2001-2004:	Alternate Councilor, Division of Computers in Chemistry, American Chemical Society
2007 – 2013	Member, Executive Committee, Division of Chemical Information, ACS.
2014	Member, Organizing Committee. In silico Drug Discovery Conference, NCBC, RTP, NC Dec 3-4
2014-present	Co-chair, Scientific Advisory Board, Skoltech, Moscow, Russia

Journals Refereed for:

Journal of the American Chemical Society.
Journal of Chemical Information and Computer Science (current name: Journal of Chemical Information and Modeling)
Journal of Computational Chemistry.
Journal of the Computer-Assisted Molecular Design.
Journal of Molecular Biology
Journal of Molecular Recognition.
Journal of Theoretical Biology
European Journal of Medicinal Chemistry
Molecular Pharmacology.
Nature Medicine.
Protein Engineering.
Proteins: Structure, Function, and Genetics.

Professional Service:

Associate Editor, Journal of Chemical Information and Modeling, 2015-
NIH Study Sections (various, 4 meetings), 2015
NIH Study Sections (various, 4 meetings), 2014
Member, senior scientist search committee, EPA (two searches in 2014)
NIH special Study section meetings (June, Oct, Dec – 2013)

Chair, IMST-11 NIH Study Section, 2010-2011

Associate Chair, Cheminformatics and QSAR Society, 2005-to date.

Expert Representative of the International Council on Animal Care and Protection (ICAPO)at OECD, Paris, 2009 – 2011.

Associate Editor, Cell Biochemistry and Biophysics, 1995-to date.

Member, Editorial Board, Journal of Computer Aided Drug Design, 1999 – 2007; 2012 - present.

Member, Editorial Board, Perspectives in Drug Discovery and Design Journal, 1999 – to date.

Member, Editorial Board, Journal of Chemical Information and Modeling, 2005 – 2012

Permanent Member, BDMA Study Section, 2006 – 2010.

Member, Editorial Board, Journal of Molecular Graphics and Modeling, 1998 – 2005;.

Chair, Organizing Committee for the North Carolina Symposium on Molecular Modeling: Integration of Theory with Experiment, Research Triangle Park, NC, October 1993.

Member, Advisory Board, Molecular Modeling Conference-94, New Brunswick, NJ, October 1994.

Session Chair (Session on "Successful applications in structure-based design"), Gordon Research Conference on QSAR, Tilton, NH, August 1995.

Session Chair (Session on "Variable Selection and Novel QSAR Methods"), Gordon Research Conference on QSAR, Tilton, NH, July 1999.

Session Chair (Session on Molecular Dynamics and Free Energy Simulations), 212th American Chemical Society Meeting, Orlando, FL, August 25-30, 1996.

Ad-hoc member, NIEHS Committee on Tenure and Promotions, 1996

Ad-hoc member, NIH panel on AIDS, 1997

External Reviewer, NSF, 1997.

Member, NSF ITR Study Section, 2002.

Co-Chair, IBC Research Conference on Chemo*Bioinformatics, San Diego, CA, 2001.

Co-Chair, Session on Rational Design of Chemical Libraries: From Hits to Leads to Drugs. ACS National Meeting, San Diego, CA., 2001

Member, NIH Special Study Section on SBIR (SSS-6), 1998 – 2006.