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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-present K.H. Lee Distinguished Professor and Associate Dean for Data and Data Science, UNC Eshelman School of Pharmacy, UNC- Chapel Hill
2016-present Chief Domain Scientist, Renaissance Computing Institute (RENCI), UNC
2012-present Member, Lineberger Comprehensive Cancer Research Center
2008-present Adjunct Professor**,** Department of Computer Science, UNC-Chapel Hill.
2004 –present Full Professor, Division of Medicinal Chemistry and Natural Products, UNC Eshelman 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.
1991-present Director, Laboratory for Molecular Modeling, Division of Medicinal Chemistry and Natural Products, School of Pharmacy, UNC- Chapel Hill (primary appointment).
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
1997-2004 Associate Professor, Division of Medicinal Chemistry and Natural Products, School of Pharmacy, UNC- Chapel Hill
1991-1997 Assistant Professor, Division of Medicinal Chemistry and Natural Products, School of Pharmacy, 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.

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2. **Tropsha, A**. Uncommon Data Sources for QSAR Modeling. In: Applied Chemoinformatics: Achievements and Future Opportunities. T. Engel and J. Gasteiger, Eds., **2018**, Wiley-VCH Verlag GmbH & Co.
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10. **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.
11. **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**.
12. 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)
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15. **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.
16. **Tropsha, A**. Application of Predictive QSAR Models to Database Mining. In: *Cheminformatics in Drug Discovery*, T. Oprea, Ed., Wiley-VCH, **2005**, pp. 437-455.
17. **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.
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32. Braga RC, Alves VM, Muratov EN, Strickland J, Kleinstreuer N, **Tropsha A**, Andrade CH. Pred-Skin: A Fast and Reliable Web Application to Assess Skin Sensitization Effect of Chemicals. *J Chem Inf Model*. **2017** May 22;57(5):1013-1017. doi: 10.1021/acs.jcim.7b00194.
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Invited Oral Presentations

INVITED LECTURES AND SEMINARS:

Dec 2019	UNC-SAS meeting, UNC-CH: Statistical modeling of drug discovery pipeline
Nov 2019	CompMed Symposium, UNC-CH: Testable Predictions of Chemical Bioactivity and Toxicity with Machine Learning Approaches
Oct. 2019	RAU, Yerevan, Armenia*: Biomedical Data Science: From Big Data to Small Molecule Drug Discovery and Repurposing*
Oct 2019	International Conference, Yerevan, Armenia: *Curated Data + Rigorous Validation = Predictive Science*
Oct. 2019	FDA, Little Rock, AR*: Progress and Challenges in the use of in silico Methods in Regulatory Science*
Sep. 2019	AI and Robotics Conference, Shenzhen, China: Biomedical Knowledge Graph Mining and AI Approaches to Drug Discovery
Aug 2019	ACS national meeting, San Diego, CA: How visualization helps with designing novel chemicals and materials with the desired properties
Aug 2019	SAS, RTP: *Application of AI and Machine Learning Methods to the Discovery of New Chemicals with the Desired Properties*
July 2019	EPA, RTP: *Curated Data + Rigorous Methods = Predictive Science*
July 2019	ESMEC symposium, Urbino, Italy: *AI-driven design of novel, synthetically feasible bioactive compounds*
June 2019	*NAS symposium, Washington, DC: Issues with reproducibility and replicability*
June 2019	Biovia User Conference, San Diego, CA: *Data Governance and Model Development Guidelines for de novo Drug Discovery and ADMET Property Assessment*
May 2019	*CARTA Meeting, RTP, NC: Big data, slow algorithms, and the need for fast decisions*
May 2019	EWDD 2019, Sienna, Italy: *Application of Text Mining and Artificial Intelligence Approaches to Drug Discovery and Repurposing*
Apr. 2019	Univ of Kentucky, Louisville, KY. *Biomedical Knowledge Mining and AI-driven Approaches for Drug Discovery*
Mar. 2019	KAUST, Saudi Arabia, Machine learning, text mining, and AI approaches for drug discovery and repurposing
Mar. 2019	NCSU, Chemistry, Raleigh, NC: *Text mining, machine learning, and AI approaches for drug discovery and repurposing*
Feb. 2019	Pistoia Alliance, Webinar: *Machine learning, text mining, and AI approaches for drug discovery and repurposing*
Jan. 2019	Penn State University, Hershey, PA. *Application of text mining and AI approaches to drug discovery and repurposing*
Nov. 2018	RASA meeting, Washington DC. *Novel Artificial Intelligence Approaches for de novo Drug Design*
Oct. 2018	NCI Cancer Nanotechnology Alliance Meeting, Washington, DC. *E-NanoBook Demonstration*
Sept. 2018	22nd European Symposium on Quantitative Structure-Activity Relationahip, Thessaloniki, Greece. *Long live QSAR*

Sep 2018 BASF, RTP. *Applications of machine learning and artificial intelligence to targeted molecular design*

Sep 2018 Samsung Corporation, Seoul, Korea. *Materials Informatics: Emerging AI and Machine Learning Approaches for Designing Novel Materials with the Desired Properties*

Aug 2018 ACS Meeting, Boston, MA. *Reminiscing about the future of QSAR*.

July 2018 Genetech, San Francisco, California. Discovery and design of novel bioactive compounds using uncommon knowledge sources and targeted library generation tools

June 2018 12th ISOPS Conference, Ankara, Turkey. *Application of Text Mining Approaches to Drug Discovery*

June 2018 6th International Workshop on Chemoinformatics. Strasbourg, France. *Applications of machine learning and artificial intelligence to designing chemicals and materials with the desired properties.*

June 2018 Universal Display Corporation, Ewing, NJ. *Applications of machine learning and artificial intelligence to designing chemicals and materials with the desired properties.*

June 2018 ACS Green Chemistry Conference, Portland, OR. *A Perspective and a New Integrated Computational Strategy for Skin Sensitization Assessment*

May 2018 1st French-Israel Cheminformatics Workshop, Bar Ilan University, Tel Aviv, Israel. *Discovery and design of novel bioactive compounds by mining uncommon and diverse knowledge sources*

Apr. 2018 Institute of Bimedical Chemistry, Moscow, Russia. *Splendors and miseries of chemical alerts*

Apr. 2018 3rd International School Seminar for Empirical to Predictive Chemistry, Kazan, Russia. *Social & professional media mining for drug discovery*

Mar. 2018 American Chemical Society, New Orleans, Louisiana. *Design of property-biased chemical libraries using artificial intelligence approaches*

Mar. 2018 Carolina Nanoformulation Workshop, University of North Carolina at Chapel Hill, Chapel Hill, NC. *Computational modeling of drug loaded nanodelivery systems*

Jan. 2018 University of Arkansas, Fayetteville, AK. *Uncommon data sources and tools for modeling chemical bioactivity*

Dec. 2017 University of British Columbia, Vancouver, BC. *Drug repurposing and design using text mining seminar and approaches*

Dec. 2017 IBM, San Jose, CA. *Drug repurposing and design using text mining approaches*

Oct. 2017 NCI Alliance for Nanotechnology in Cancer Principal Investigators Meeting, Bethesda, MD. *Alliance 2016 Pilots: eNanoBook and data sharing*

Oct. 2017 2017 Annual International Society of Expsoure Science, Cary, NC. *QSAR-based methods and tools to support HTP risk assessment*

Sept. 2017 Rutgers University, Camden, NJ. *Application of text mining and data mining to drug discovery and repurposing*

Aug. 2017 American Chemical Society 254th National Meeting, Washington, DC. *Applications of machine learning to materials and chemical property prediction*

July 2017 3rd Kazan Summer School on Cheminformatics, Kazan, Russia. *Structural alerts for promiscuity and toxicity: the good, the bad, or the ugly?*

July 2017 Gordon Research Conference, West Dover, VT. *Computer aided drug design*

June 2017 Gordon Research Conference, West Dover, VT. *Cancer nonotechnology*
May 2017 Genetics and Environmental Mutagen Society (GEMS), Durham, NC. *Data Science Nanomaterials*
Apr. 2017 American Chemical Society National Meeting, San Francisco, CA. *What works best for predicting human skin sensitization potential of chemicals: in vitro data or in silico models*
Apr. 2017 American Chemical Society National Meeting, San Francisco, CA. *Mining protein interactions from biomedical literature using semantic similarity*
Apr. 2017 Roswell Park Cancer Institute, Buffalo, NY. *Rational drug design*
Apr. 2017 Materials Research Society, Phoenix, AZ. *Materials Informatics: computer-aided design of novel materials with the desired electronic and physical properties*
Jan. 2017 Stanford University. *Data science of everything: from small molecules to big data*
Dec. 2016 RTP-180: Alarms about Structural Alerts
Dec. 2016 Pfizer, Groton, CT. *Data Science of QSPR Modeling*
Nov. 2016 Big Data to Knowledge (BD2K) All Hands Meeting and Open Data Science Symposium, Bethesda, MD. *Hypothesis fusion to improve the odds of successful drug repurposing*
Sept. 2016 21st European Symposium on Quantitative Structure Activity Relationship, Verona, Italy. *Improving drug loading into polymeric micelles by cheminformatics tools*
Sept. 2016 2nd Internationl Scientific Conference-Science of the Future, Kazan, Russia. *Computer modeling of drug delivery systems*
Sept. 2016 Mendeleev Congress on General and Applied Chemistry, Ekaterinburg, Russia. *Data curation is critical for the success of modeling research*
Sept. 2016 Mendeleev Congress on General and Applied Chemistry, Ekaterinburg, Russia (Plenary Lecture). *Cheminformatics Has its Hands in all Human Affairs*
Aug. 2016 American Chemical Society Fall Meeting, Washington, DC. *Contrasting polypharmacology and pan-assay interference compounds*
Jul. 2016 American Association of College of Pharmacy Annual Meeting, Anaheim, CA. Data Science in Pharmacy: from small molecules to Big Data
June 2016 Strasbourg Summer School in Chemoinformatics, Strasbourg, France. *Alarms about structural alerts*
June 2016 Renaissance Computing Institute Data Science Meeting. *The unifying power of data science: a journey from small molecules to big data*
Apr. 2016 University of Buffalo, Buffalo, NY. *The data science of everything from small molecules to big data*
Apr. 2016 University of Buffalo, Buffalo, NY. *Fundamentals of QSAR modeling: basic concepts and applications*
Mar. 2016 American Association of Colleges of Pharmacy (AACP) Reseach Fellows Meeting, Washington, DC: *The unifying power of data science: a journey from small molecules to big data*
Mar. 2016 CBMC Division. *Data science of everything: from small molecules to big data*
Mar. 2016 UNC Workshop on Nanodelivery (NanoDDS): QNTR. *Computer modeling of nanomaterials and liposome-based drug delivery systems*
Mar. 2016 UNC-Health Informatics Program. *Gheminformatics-aided pharmacovigillance: application to Stevens-Johnson Syndrom*
Jan. 2016 Interagency Coordinating Committee on the Validation of Alternative Methods (ICCVAM) Community of Practice Webinar *Fundamentals of QSAR modeling: basic concepts and applications*
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. NIH AG059428-01A1. Drug Repurposing for Alzheimer's Disease. Total Direct Requested 2.5M.
2. R01AG059428-01A1: ARAGORN: Autonomous Relay Agent for Generation of Ranked Networks. 1/13/20120 – 1/12/2024;

Currently funded research grants (Principal Investigator).

1. NIH 1OT2TR003441-01: Total Cost: TBD
2. NIH 1U01CA207160-01. *Drug Repurposing for Cancer Therapy: From Man to Molecules to Man. 09/01/16-08/31/20.* Total Cost: $1,264,276
3. NIH 1R01GM114015-01 (coPI with Dr. Nikolay Dokholyan). Integrating cheminformatics and molecular simulations for virtual drug screening. 08/15/2016 – 05/31/2021. $93K/year to Tropsha lab.
4. NIH/NCATS 1OT3TR002020-01. *Biomedical Data Translator Technical Feasibility Assessment and Architecture Design (shared PI with Dr. Stanley Ahalt). 09/24/16-03/31/2020* Total Cost: $454,336
5. NIH/NCATS 1OT2TR002514-01. Biomedical Data Translator Technical Feasibility Assessment of Reasoning Tool: University of North Carolina at Chapel Hill. 01/05/2018 – 12/31/2020. Total Cost: $1M.
6. Office of Naval Research N00014-16-1-2311. *Materials Informatics Platform for Property Prediction. 02/04/16-05/31/20*. Total cost: $300,000
7. Eshelman Institute for Innovation. Elucidating the effect of bariatric surgery on diabetes progression using patient data. 7/1/2018-6/30/2020. Total Direct Cost $200K.
8. Pharmalliance. *PharmSim Program Synchronization across the PharmAlliance to Enhance Education, Practice and Research in Pharmacy.* 01/20/2016-1/20/2017. Total cost: $14,000

9. University of North Carolina ROI/IPG. *Data Science: Infohub for Rare Diseases*. 07/01/2017-06/30/2020. Total direct cost: $326,438 to UNC.

Currently funded research grants (Co-Investigator).

10. NIH 1OT3OD025464-01. *A Collaboration for the NIH Data Commons* (Investigator; PI Stanley Ahalt). 09/30/2017-06/30/2020. Total cost: $1,224,574
11. NIH 1OT3HL142479-01. *A Collaboration for the NIH Data Commons (Investigator; PI Stanley Ahalt).* 09/30/17-09/29/2020. Total cost: $1,200,000
12. NIH/NCI: Nano Approaches to Modulate Host Cell Response for Cancer Therapy; Project 4 title: High Capacity Polymeric Micelle Therapeutics for Lung Cancer. Role: Project 4 Investigator; Project 4 Direct Costs: $343,636
13. DOD DM170665 Medical Learning Through Machine Learning (Investigator; PI J. Heneghan) 9/01/2018 – 9/29/2020 .36 cal.

Completed projects.

14. NIH/NCI *Supplement: Nanobook: A Tool to Facilitate Data Collection and Deposition into Nanomaterial Databases (Project Lead).* Major Grant*: Nano Approaches to Modulate Host Cell Response for Cancer Therapy*; *08/01/2016 – 07/31/2017. Total cost: $149,653.*
15. Eshelman Institute for Innovation. *A Virtual Environment to Enhance Education, Practice, and Research in Pharmacy*. *10/1/2015 – 9/30/2018*. Total cost: $1,994,776
16. PharmAlliance. *AI-driven Design of Kinase Inhibitors with Selective Polypharmacology for the Treatment of Chordoma*. 12/01/2017-11/30/2018. Total cost: $25,331
17. Pfizer, Inc. *Development of a State-of-the-Art Model of Free Energy of Fusion to Facilitate Accurate Solubility Predictions in Any Solvent System. 09/15/16-09/14/17*. Total cost: $117,287
18. 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.
19. ChemBench: the Integrated Web Portal to Accelerate Cheminformatics and Chemical Genomics Research. Total direct (per year): Direct cost $190,000/year, **NIH**, R01 GM 096967-01A1. (10%).
20. ABI Program: Innovation: Synergistic application of cheminfomatics and computational geometry approaches for modeling protein-protein interactions. **NSF** 10-567 Advances in Biological Informatics. (10%) Direct cost: $200,000/year. 8/01/12-7/31/16.
21. 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).
22. NC TraCS. delAQUA – Computer-Assisted Drug Solubilization Platform (4DR11404; 50K); PI: Sasha Kabanov; 6/1/2015 – 6/1/2016
23. 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; subcontract PI: Tropsha). 9/15/2014 – 12/15/2015, Total Cost to UNC: 350K
24. Computer-Aided Design of Nanomaterials with the Desired Bioactivity and Safety Profiles. **Semiconductor Research Corporation**. Y502164 (3%). Total cost: 125,600/year. 1/1/2012 – 12/31/2014
25. Predictive QSAR models of hepatotoxicity. **EPA RD 83499901** (10%). Direct Cost: 170K/year. Dates: 5/1/2011 – 4/30/2014.
26. Disposition of Flavonoids via Metabolic Interplay. **NIH NOT-GM-08-130**. 08/01/10-07/31/13. Direct cost to Tropsha lab: $39,930/year.
27. 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/year direct to Tropsha Lab)

28. 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)
29. 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).
30. 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.
31. Predictive ADME/Tox Modeling. **NIH 3R01CA120921-02S1** (ARRA Competitive Supplement). Dates: 08/01/2009 – 07/31/2011. Total cost: $396,640; first year direct cost $134K (ca. 80K to Tropsha lab)
32. 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).
33. Robust Computational Framework for Predictive ADMETox Modeling (15%). **NIH R21GM076059.** Dates: 6/1/06 – 5/31/11. Total direct cost $732,375.
34. Protein Structure/Function Specific Packing Motifs (10%). **NIH**. Dates: 8/1/06-7/30/11. Total direct cost - $760,000.
35. 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.
36. Developing Novel Cheminformatics Tools to Accelerate the Search for Cancer Therapeutics. UCRF (100K total and direct). Dates: 3/1/2009 – 2/28/2011.
37. 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
38. 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).
39. 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)
40. 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)
41. Carolina Exploratory Center for Cheminformatics Research (15%). **NIH P20HG003898**. Dates 9/1/05-8/31/09. Total direct cost: $750,000
42. Carolina Center for Exploratory Genetic Analysis. **NIH P20-RR20751** (Reed). Co-investigator (5%). Dates: 6/1/2004 – 5/31/2006. Total Direct Cost: 750K.
43. Novel Computational Tools to Identify Residue Motifs from Protein Graphs (Wang). NSF 0523875 Co-investigator (5%). Dates: 10/1/05 – 9/30/08.
44. Systematic Discovery of Automatic Gene Regulation Modules in Cell Cycle Dynamics (4%). Elsa A. Pardee Foundation, total first year direct cost $54,000
45. Computational Geometry for Structural Biology and Bioinformatics (Edelsbrunner). Co-PI (5%). **NSF CCR-0086013**.
46. 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.
47. 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.
48. Predictive QSAR Modeling (Minority Supplement) – PI. **NIH. R01GM066940-01A1S1**. $26,842 direct cost. Dates: 8/15/03-8/14/04.
49. 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.

50. 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.
51. 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.
52. 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.
53. 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.
54. 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: $218,000, current year direct cost: $71,129.
55. 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.
56. 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.
57. 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.
58. 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.
59. 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.
60. 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.
61. 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.
62. Hoechst Celanese Corporation/UNC-CH Research Partnership. Molecular Simulations of β-amiloid peptides. Dates: July 1, 1995-June 30 1996. Amount Funded: $25,000.
63. 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.
64. **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.
65. 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.
66. 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.

67. 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.
68. 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.
69. 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.
70. 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.
71. 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.
72. 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
73. 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)
Contract Research Support, Pfizer Inc, 2016-2017 ($117K0

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
- Dr. Regina Politi, Postdoctoral Fellow, 2012-2016. Current Position: Data Scientist, BCBS
- Dr. Tigran Abramyan, Postdoctoral Fellow, 2018 - 2019 *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. Asst. Prof from 2011.
- Dr. Olexander Isayev, Research Asst. Prof, 2013 – 2019.
- Dr. Stephen Capuzzi, Postdoctoral Fellow, 2018 – 2019
- Dr. Vinicius Alves, Postdoctoral Fellow, 2018 – 2019
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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, NCATS, NIH, Bethesda.
Bala Krishnamoorthy	Ph.D., Operations Research, 2004. Present position: Assoc. 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: Assoc. 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: Office Staff, Eileen Wang, LLC.
Ruchir Shah	Ph.D., Material Sciences, 2006. Thesis: *Computational analysis of protein function and protein-protein interactions*. Present position: Principal and Senior Bioinformatics Manager, SRA International, 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.* Present position: Asst. Prof, UT Tyler.
Kun Wang	PhD., Medicinal Chemistry, 2009. Thesis: *Classifier Design to Improve Pattern Classification and Knowledge Discovery for Imbalanced Datasets.* Present position: Unknown.
Amy 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*. Present position: unknown
Rima Hajou	PhD., Medicinal Chemistry, 2010. *In Silico Strategies to Study Polypharmacology of G-Protein-Coupled Receptors*. Present Position: Research Scientist, Elsevier, Boston.
Chris Grulke	PhD., Medicinal Chemistry, 2011. *Development and Extension of Cheminformatics Techniques for Integration of Diverse Data to Enhance Drug Discovery.* Present Position: Research Scientist, EPA.
Jui-Hua Hsieh	PhD., Medicinal Chemistry, 2011. *Cheminformatics Approaches to Structure Based Virtual Screening: Methodology Development and Applications*. Present Position: Research Scientist, NIEHS.
Hao Tang	PhD., Biochemistry & Biophysics, 2011 *Prioritizing Small Molecules for Drug Discovery or Chemical Safety Assessments from Ligand- and Structure-Based Cheminformatics Approaches.*

	Present Position: Assistant Professor at **UT Southwestern** Medical Center
Liying Zhang	PhD., Medicinal Chemistry, 2011. *Development and Application of Cheminformatics Approaches to Facilitate Drug Discovery and Environmental Toxicity Assessment.* Present position: Senior Scientist, Pfizer.
Man Luo	PhD., Medicinal Chemistry, 2011. *Cheminformatics Modeling of Diverse and Disparate Biological Data and the Use of Models to Discover Novel Bioactive Molecules.* Present position: Principal Scientist, Johnson & Johnson
Guiyu Zhao	PhD., Medicinal Chemistry, 2011. *The QSARome of the Receptorome: Quantitative Structure-Activity Relationship Modeling of Multiple Ligand Sets Acting at Multiple Receptors.* Present Position: Function Head, Medical Data Science, Hua Medicine Inc.
Tanarat Kietsakorn	MS., Medicinal Chemistry, 2011. *Protein Function Prediction using Family-specific Structural Motifs.* Present Position: unknown
Dongqiuye Pu	MS, Molecular Pharmaceutics, 2012 *Quantitative Structure-Toxicity Relationship Modeling of Organic Compounds and Nanoparticles.* Present Position: unknown
Tony Wu	PhD., Biomedical Engineering, 2012. *Novel Cheminformatics Methods for Modeling Biomolecular Data in High Dimension Low Sample Size (HDLSS) Chemistry Space.* Present position: Application Specialist at Linguamatics, Boston
Yen Low	PhD, Environmental Science and Engineering, 2013. *Toxicity Prediction Using Multi-disciplinary Data Integration and Novel Approaches.* Current position: Lead ML Scientist at Rally Health
Petro Borisov	PhD, Statistics and Operations Research (co-advised with Steve Marron), 2013. Statistical Methods in Chemoinformatics. Current Position: Research Scientist, SAS Institute
Stephen Bush	PhD, Bioinformatics and Computational Biology, 2013. Novel Cheminformatics Approaches for Modeling Protein-Protein Interactions. Current Position: Principal Scientist, Tempus, Chicago
Andrew Fant	PhD, Medicinal Chemistry, 2015. The effect of data curation on the accuracy of quantitative structure-activity relationship models. Current position: Research Scientist, Leidos.
Stephen Capuzzi	PhD, Medicinal Chemistry, 2018. Predictive Cheminformatics Analysis of Diverse Chemogenomics Data Sources: Applications to drug discovery, assay interference, and text mining.
Sherif Farag	PhD, Bioinformatics, 2019: Computational Design of Novel Non-Ribosomal Peptides
Kyle Bowler	MS, Pharmaceutical Sciences; 2019: Cheminformatics Analysis and Computational Modeling of Detergent-Sensitive Aggregation

Current:

Andrew Thieme	PhD, Pharmaceutical Sciences, 2022 (anticipated)
Daniel Korn	PhD, Computer Science, 2022 (anticipated)
Joshua Hochuli	PhD, Bioinformatics, 2023 (anticipated)

C. Visiting Fellows, rotation, and honors students:

Mar. 2018-Mar2019. Joyce Borba, visiting grad student, Federal University of Goiás, Brazil

Oct. 2016 – April 2017: Maria Popova, visiting graduate student, Skoltech, Russia
Oct-Dec 2016: Elena Tutubalina, visiting research scientist, Kazan Federal University, Kazan, Russia
2014-2016. Vinicius Alves, visiting graduate student, Federal University of Goiás, Brazil
2014: Mary La, PY3, School of Pharmacy
2014: Hugh Heldenbrand, PY1, School of Pharmacy

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 Pharmacoinformatics and Data Science, 2016-present
Chief Domain Scientist in Data Science, Renaissance Computing Institute, 2016-present

Associate Dean for Research and Graduate Education, 2011 – 2015.
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;
2011-2015: Member, UNC Conflict of Interest Committee;
2013 – present: University Health Informatics Committee
2012-present: Member, CTSA steering committee
2017-2017 Chair, Campus Data Science Initiative Committee, UNC
2017-2018 Chair, Search committee for Director, Catalyst for Rare Diseases

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); graduated Fall 2016
Reed Jacob (Biochemistry and Biophysics): expected I Spring 2017.

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:

Member, NIH Special Advisory Panel to review Laboratory for Chemical Biology, NCI
Chair, Special NIH Study Section on Digital Biomedical Data Curation, Feb 2017.
Associate Editor, Journal of Chemical Information and Modeling, 2015-
NIH Study Sections (various, 3 meetings), 2016
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.