JINHUA ZHANG, Ph. D.

43114 30th Street West # 207
Lancaster, CA 93536, USA
zhangjinhua@gmail.com, (661) 236-1208

HIGHLIGHTS OF QUALIFICATIONS

- Experienced computational chemist with expertise in computational drug discovery, medicinal chemistry, statistical modeling, machine learning, data mining, data analysis, and database management
- Proven ability to apply highly advanced simulation and modeling strategies to drug development in a creative and resourceful manner
- Extensive experience in design and developing state-of-the-art scientific software for drug discovery
- Demonstrated ability to solve difficult problems independently as well as to work effectively with coworkers in a team-oriented environment
- Good communication skills complemented by a keen analytical ability

EDUCATION

- Ph.D. in Chemistry, Texas A&M University (1999)
- M.S. in Information and Systems Science, Carleton University, Canada (2003)
- B.S. in Organic Chemistry, Wuhan University, China (1986)

PROFESSIONAL EXPERIENCE

Simulations Plus, Inc. Lancaster, California, USA (2006 – present)
Senior Scientist II (2011-present), Senior Scientist (2006-2011): Development and deployment of computational prediction models for drug absorption, distribution, metabolism, excretion, and toxicity. Scientific programming for drug discovery modeling software *ADMET Predictor™*

- **Development of computational prediction models for *ADMET Predictor*™ software:**
  - Substrate prediction models for Cytochrome P450 1A2, 2A6, 2B6, 2C8, 2C9, 2C19, 2D6, 2E1, 3A4
  - Metabolic sites prediction models for substrates of Cytochrome P450 2C9, 2D6, and 3A4
  - Metabolic-site-specific kinetic parameters (K_M, V_{max}, CL_{int}) prediction models for drug metabolism mediated by Cytochrome P450 1A2, 2C9, 2C19, 2D6, and 3A4
  - Inhibition prediction models for Cytochrome P450 1A2, 2C9, 2C19, 2D6, and 3A4
  - P-gp substrates and inhibition prediction models
  - Human HIV-1 Integrase inhibition prediction models for anti-AIDS drugs discovery
  - Supersaturated tendency prediction model for drugs in aqueous solutions
  - Corneal permeability prediction model
  - Henry's law constant prediction model for volatile compounds
  - ADMET risk for multi-objective drug development based on the analysis of predicted ADMET properties of World Drug Index (WDI) data set
  - Structure-activity landscape index (SALI) in *ADMET Predictor™* for evaluating the performance of QSAR models
- **Scientific research for pharmaceutical studies:**
  - Research services for providing lead optimization using computer-based molecular design and *in silico* ADMET models for customers' drug candidates
  - Investigated the modeling of carcinogenicity and Ames mutagenicity data in the project collaboration with US Food and Drug Administration (FDA)
  - Investigated the modeling of environmental toxicity models against *Tetrahymena pyriformis*

- Developed *plasmodium falciparum* dihydroorotate dehydrogenase (*Pf*DHODH) inhibition models for anti-malarial drugs discovery project
- Developed the buccal permeability prediction model
- Developed the logP prediction model for millamolecular drugs
- Developed the best model for predicting intrinsic solubility in the contest of the *Journal of Chemical Information and Modeling (2008)*
- Evaluated various statistic as measures for classification modeling with highly imbalanced data

University of Ottawa, Department of Chemistry, Canada (2006)
Research associate
- Applied structure based empirical and quantum molecular descriptors to high-throughput system and QSAR models to aid the design of novel catalysts

University of Erlangen-Nurnberg, Computer-Chemistry Center, Germany (2003 – 2005)
Research associate: Research in cheminformatics and computational drug discovery. A scientific programmer of cheminformatics software *MOSES* (Molecular Structure Encoding System).
- Developed acidic-site-specific pK_a prediction models using molecular and atomic charge descriptors
- Developed new atomic descriptors modeling the electronic inductive effect
- Designed and implemented the QSAR modeling and virtual screening tool VANESSA
- Designed and implemented an object-oriented back-propagation neural network modeling module for *MOSES* software
- Contribution to the development of wavelet transformation module for multivariate chemical data analysis.

Carleton University, Department of System and Computer Engineering, Canada (2000 – 2002)
Graduate research assistant
- Research on UML (United Modeling Language) and system performance of distributed software systems with simulation and modeling
- Teaching assistant in operating systems, object-oriented programming classes.

University of Ottawa, Department of Chemistry, Canada (1999 – 2000)
Postdoctoral research fellow
- Investigated the catalytic properties of organometallic compounds grafted silica with quantitative FT-IR and solid state NMR spectroscopy.

Texas A&M University, Chemistry Department (1993 – 1999)
Graduate research assistant
- Ph.D. dissertation studies on characterizing surface acidity of catalysts with multiple solid state NMR spectroscopy and theoretical computations.
- Instructor of organic chemistry laboratories.

Zhengzhou Institute of Light Industry, Department of Chemical Engineering, China (1986 – 1993)
Lecturer
- Instructor of organic chemistry and laboratories.

AFFILIATIONS AND PROFESSIONAL ACTIVITIES

- American Chemical Society, member (since 1994)
- Southwest Catalysis Society, member (since 1995)
- Session chair, 6th Annual Congress of International Drug Discovery Science and Technology, Beijing, China, Oct 20, 2008
- Roundtable moderator, HIV Inhibitors Exploring Today's Most Promising Targets, San Diego, CA, April 8, 2009
- Reviewer: PLOS Computational Biology

HONORS AND AWARDS

- Phi Lambda Upsilon (1995), Texas A&M University
- Ontario Graduate Scholarship in Science and Technology (2001), Canada

PUBLICATIONS

"Busting the Black Box Myth: Designing Out Unwanted ADMET Properties with Machine Learning Approaches." R. Fraczkiewicz, D. Zhuang, **J. Zhang**, D. Miller, W. S. Woltosz, M. B. Bolger. CICSJ Bulletin, 27, No. 4, 96 (2009) (Division of Chemical Information and Computer Sciences, the Chemical Society of Japan)

"Prediction of pK_a values for Aliphatic Carboxylic Acids and Alcohols with Empirical Atomic Charge Descriptor." **J. Zhang**, T. Kleinöder and J. Gasteiger, *J. Chem. Inf. Modeling,* 46, 2256 (2006)

"NMR and Theoretical Study of Acidity Probes on Sulfated Zirconia Catalysts." J. F. Haw, **J. Zhang**, K. Shimizu, T. N. Venkatraman, D. Luigi, W. Song, D. H. Barich and J. B. Nicolas. *J. Am. Chem. Soc.* 122, 12561 (2000)

" NMR and Theoretical Study of Acid Sites Formed by Adsorption of SO_3 onto Oxide Surfaces." J. Zhang, J. B. Nicolas and J. F. Haw, *Angew. Chemi*, 112, 3440 (2000)

"Modeling of Benzene Adsorption in Metal-Exchanged Zeolites by Calculation of ^{7}Li Chemical Sifts." D. H. Barich, T. Xu, **J. Zhang** and J. F. Haw*, Angew. Chemi international ed.*, 37, 2530 (1998)

"^{13}C NMR Observation of Photoproducts in Zeolites and Their Further Reactions on Acid Sites." **J. Zhang**, T. R. Krawietz, T. W. Skloss and J. F. Haw, *J. Chem. Soc. Chem. Commun.,* 685 (1997)

"Imine Chemistry in Zeolites: Observation of gem-Amino-Hydroxy Intermediates by In Situ ^{13}C and ^{15}N NMR." T. Xu, **J. Zhang** and J. F. Haw, *J. Am. Chem. Soc.,* 117, 3171 (1995)

"A Report of Persistent Allyl Cation on HZSM-5 Zeolite Was Due to Propanal." T. Xu, **J. Zhang** and J. F. Haw, *J. Chem. Soc. Chem. Commun.,* 2733 (1994)

"Studies of Porphyrin Compounds III. Synthesis of Bridged Crowned Porphyrines and Their Cobalt(II) Complexes." S. Xia, Z. Jiang, H. Ke, **J. Zhang** and S. Huang, *J. Wuhan University, Natural Science Ed.*, 79 (1989)

BOOK CHAPTERS

"Performance Analysis with the UML SPT Profile". D. C. Petriu, **J. Zhang**, G. Gu and H. Shen, pp. 205-224. In: *Model-Driven Engineering for Distributed and Embedded Systems*, Eds. J. Champeau, J. P. Babau and S. Gerard, HERMES Science Publishing Ltd., London, 2005

ORAL PRESENTATIONS

"The Development of *in silico* Models to Predict K_M, V_{max} for CPY450 Isozymes". 7th Annual Congress of International Drug Discovery Science and Technology, Shanghai, China, Oct 22-25, 2009

"In silico studies of ADMET properties". Boehringer-Ingelheim, Canada Ltd. August 14th, 2009, Laval, Canada

"Prediction of HIV-1 Integrase Inhibitory Activity." Cambridge Healthtech Institute (CHI) conference, HIV Inhibitors Exploring Today's Most Promising Targets, San Diego, CA, April 7-8, 2009

"Predicting Kinetic Parameters for Substrates of Human Cytochrome P450." ACS 237th National Meeting, Salt Lake City, UT, March 26, 2009

"in silico Studies of ADMET Properties in Early Drug Discovery." 6th Annual Congress of International Drug Discovery Science and Technology, Beijing, China, Oct 18-22, 2008

"Prediction of pK_a with PETRA Atomic Charge Descriptors." Organon Pharmaceuticals Inc., Glasgow, UK, March 31, 2005

POSTER PRESENTATIONS

J. Zhang, R. Fraczkiewicz**,** M. Walderman, M. Lawless, and R. D. Clark, "Predicting Metabolic-site-specific Kinetic Parameters for CYP2D6-mediated Drug Metabolism", ACS 245th National Meeting, New Orleans, AB, April 7-12, 2013

A. Lee, M. S. Lawless, **J. Zhang**, R. Fraczkiewicz**,** M. Walderman, R. D. Clark, and W. S. Woltosz, "Estimating Confidence in Toxicity Predictions", SETAC North America 33rd Annual Meeting, Long Beach, CA, Nov. 11-15, 2012

M. Walderman, R. Fraczkiewicz**, J. Zhang**, and R. D. Clark, "*In Silico* Metabolite Prediction Using Artificial Neural Network Ensembles", Cambridge Healthtech Institute (CHI) conference, San Diego, CA, April 17-19, 2012

M. Lawless, **J. Zhang**, D. Zhuang, E. Matthews, M. Walderman, R. Fraczkiewicz, "Controlling Specificity and Sensitivity in Artificial Neural Networks Ensembles (ANNE) Classification Models", ACS 243rd National Meeting, San Diego, CA, March 25-29, 2012

R. Fraczkiewicz**,** M. Walderman, D. Zhuang, **J. Zhang**, A. C. Lee, R. D. Clark, and W. S. Woltosz, "Toxicity Modeling Done Right with Artificial Neural Network Ensemble and Descriptors of Reactivity", ACS 243rd National Meeting, San Diego, CA, March 25-29, 2012

M. Waldman, R. Fraczkiewicz, **J. Zhang**, R. D. Clark, and W. S. Woltosz, "Predicting Site of Metabolism with Artificial Neural Network Ensembles", CHI's 10th Annual World Pharma Congress, Philiadelphia, PA, June 7-9, 2011

J. Zhang, R. D. Clark, R. Fraczkiewicz, M. B. Bolger, M. Waldman, and W. S. Woltosz, "Beyond Filters: ADMET Risk for Multi-objective Drug Development", ACS 241st National Meeting, Anaheim, CA, March 30, 2011

D. Miller, R. Fraczkiewicz, **J. Zhang**, M. Waldman, R. D. Clark, and W. S. Woltosz, "Novel ADMET Design Tool for Chemists", ACS 241st National Meeting, Anaheim, CA, March 28, 2011

R. Fraczkiewicz, D. Zhuang, **J. Zhang**, D. Miller, W. S. Woltosz, and M. B. Bolger, " Drug Design from a New Angle: Improving Molecule Design with Demystified ADMET Predictions", ACS 239th National Meeting, San Francisco, March 21-25, 2010

W. Woltosz, R. Fraczkiewicz, D. Zhuang, **J. Zhang**, and M. Bolger, "Structure-Property Prediction with Unbalanced Data Sets", Drug Discovery and Development Summit, Santa Fe, New Mexico, September 23-25, 2009

R. Fraczkiewicz, **J. Zhang**, M. Waldman, W. Woltosz, "Modeling Rat Liver Toxicity Signature Using Machine Learning Techniques", The First ToxCast™ Data Analysis Summit, Research Triangle Park NC, May 14-15, 2009

Z. Zhuang, **J. Zhang**, R. Fraczkiewicz, M. B. Bolger, M. Waldman, W. S. Woltosz, and K. Enslein "Inhibition Models for Cytochrome P450 1A2, 2C9, 2D6, and 3A4", ACS 237th National Meeting, Salt Lake City, UT, March 26, 2009

M. Waldman, R. Fraczkiewicz, **J. Zhang**, J. Crison, and W. S. Woltosz *"in silico* ADMET Models Using High Throughput Quantum Descriptors and Genetic Algorithms", 15th Annual ISSX North American Regional Meeting, San Diego, 2008 October 12-16

J. Zhang, R. Fraczkiewicz, M. B. Bolger, M. Waldman, W. Woltosz, and K. Enslein "Predicting Kinetic Parameters K_M and V_{max} for Substrates of Human Cytochrome P450 1A2, 2C9, 2C19, 2D6, and 3A4" 2008 2nd Asian Pacific Regional Meeting of International Society for the Study of Xenobiotics (ISSX). Shanghai, China, May 11-13, 2008

D. Miller, N. Yu, **J. Zhang**, R. Fraczkiewicz, and W. Woltosz "Strategy for the *de novo* Design and Evaluation of Drug Candidates" 2007 3rd Modern Drug Discovery & Development (M3D), San Francisco, CA, November 28-30, 2007

J. Zhang, R. Fraczkiewicz, M. B. Bolger, N. Neamati, and W. Woltosz "Quantitative Structure-activity Relationship Studies of HIV-1 Integrase Inhibitory Activity" 2007 American Association of Pharmaceutical Scientists Annual Meeting, Dan Diego, CA, November 11-15, 2007

S. Nilar, D. Zhuang, D. Miller, R. Fraczkiewicz, M. Waldman, W. Woltosz and **J. Zhang** "Classification of AMES Mutagenicity Data for Salmonella Typhimurium by SVM and ANN Modeling Techniques" 2007 American Association of Pharmaceutical Scientists Annual Meeting, Dan Diego, CA, November 11-15, 2007

T. Kleinöder, **J. Zhang**, and J. Gasteiger "Prediction of pK_a Values for Aliphatic and Aromatic Oxy-Acids and Amines with Empirical Charge" 4th Joint Sheffield Conference on Chemoinformatics, Sheffield, UK, June 18-20, 2007

J. Zhang and J. F. Haw. "Multinuclear NMR Studies of Zirconia and Sulfated Zirconia", Southwest Catalysis Society and Texas A&M University Center for Catalysis Symposium, May 21-22, 1998, College Station, Texas

J. Zhang and J. F. Haw. "Hydroxyarylation, Dealkylation, and Hydride Transfer reactions on Zeolite HUSY: An In Situ ^{13}C NMR Study", IUCCP 5th Symposium of Graduate Research in Chemistry, September 29-30, 1997, College Station, Texas

J. Zhang, T. Xu, J. F. Haw. "^{13}C MAS NMR Observation of Diphenylhalocarbenium Ions and Triphenylmethyl Cation on Zeolite HY and Aluminum Halides", Southwest Catalysis Society 1997 Symposium, April 4th, 1997, Austin, Texas

T. R. Krawietz, **J. Zhang**, T. W. Skloss, J. F. Haw. "Studies of Photochemistry on Catalysis", Thirty-seventh Experimental Nuclear Magnetic Resonance Conference, March 17-22, 1996, The Asilomer Conference Center, Pacific Grove, California