BIOGRAPHICAL SKETCH

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NAME	POSITION TITLE
Golbraikh, Alexander	Research Associate Professor
eRA COMMONS USER NAME GOLBRAIKH	

EDUCATION/TRAINING *(Begin with baccalaureate or other initial professional education, such as nursing, and include postdoctoral training.)*

INSTITUTION AND LOCATION	DEGREE *(if applicable)*	YEAR(s)	FIELD OF STUDY
Latvian State University, USSR (now Latvia)	MS	1980	Physics
Latvian Institute of Organic Synthesis, the Latvian Academy of Sciences, Riga, Latvia	PhD	1994	Chemistry
Latvian Institute of Organic Synthesis, Riga, Latvia	Post-doctoral	1995-1999	Molecular Modeling
Martin Luther University, Halle, Germany	Post-doc.	1996	Molecular Modeling
Martin Luther University, Halle, Germany	Post-doc	1997	Molecular Modeling
Orleans University, Orleans, France	Post-doc.	1998-1999	QSAR
University of North Carolina at Chapel Hill, Chapel Hill, NC, USA	Post-doc	1999-2001	QSAR, Molecular modeling

A. Personal Statement

My role in this proposal is to apply advances in applied mathematics and statistics to the molecular modeling algorithms used in Core 3 (Cheminformatics) of the proposed work. I am highly qualified to take on this role. I have a long career working at the intersection of math, statistics, chemistry, and computer science. I am currently working in the fields of computer-aided drug design and discovery, cheminformatics, **computational toxicology**, and chemical systems biology in the Tropsha lab at UNC Eshelman School of Pharmacy. The scope of my scientific interests includes also development of algorithms and software, multivariate data analysis and mathematical statistics. I am an author of more than 40 publications in the peer-reviewed scientific journals and three book chapters.

B. Positions and Honors

Professional and Research Experience

1982-1987: Engineer-Mathematician, Design Office of Mechanization and Automation, Riga, USSR
1987-1994: Research Assistant, Latvian Institute of Organic Synthesis, Riga, Latvia.
1994-1999: Research Scientist, Latvian Institute of Organic Synthesis, Riga, Latvia.
1996-1996: Postdoctoral Fellow, Martin Luther University, Halle, Germany.
1997-1997: Research Scientist, Martin Luther University, Halle, Germany.
1998-1999: Postdoctoral Researcher, Orleans University, France.
1999-2001: Postdoctoral Research Associate, Division of Medicinal Chemistry and Natural Products (MCNP), School of Pharmacy, UNC- Chapel Hill.

2001-2007: Research Assistant Professor, Division of Medicinal Chemistry and Natural Products (MCNP), School of Pharmacy, UNC- Chapel Hill.
2007-present: Research Associate Professor, Division of Medicinal Chemistry and Natural Products (MCNP), School of Pharmacy, UNC- Chapel Hill.

Honors

1978 - First place in the 1977/78 academic year competition in **mathematics** of the All-Union olympiada "The Student and the Scientific-Technical Progress."
1996 - Recipient of the DAAD (German Academic Exchange Service) Grant.

Service

Member of the American Chemical Society (since 2001).
Member of Cheminformatics and QSAR Society (since 2001).
Member of the Society of Toxicology (since 2012).
Reviewer for Journal of Chemical Information and Modeling, Journal of Medicinal Chemistry, European Journal of Medicinal Chemistry, Chemometrics, Chemistry Central Journal, Molecular Diversity, Journal of Biomedicine and Biotechnology.

C. Publications

BOOK CHAPTERS

3. **Golbraikh, A.**; Wang, X. S.; Zhu, H.; Tropsha, A. Predictive QSAR modeling: Methods and applications in drug discovery and chemical risk assessment. In: Handbook of Computational Chemistry, (Leszczynski, J., Ed.) Chapter 37, pp. 1311-1342, Springer-Verlag, Dordrecht, Heidelberg, London, New York, 2011.

2. Tropsha, A.; **Golbraikh, A**. Predictive Quantitative Structure–Activity Relationships Modeling: Development and Validation of QSAR Models. In: Handbook of Chemoinformatics Algorithms (Faulon, J.-L.; Bender, A., Eds.), Chapter 7, pp. 213-233, Chapman & Hall / CRC, London, UK, 2010.

1. Tropsha, A.; **Golbraikh, A**. Structure–Activity Relationships Modeling: Data Preparation and the General Modeling Workflow. In: Handbook of Chemoinformatics Algorithms (Faulon, J.-L.; Bender, A., Eds.), Chapter 6, pp. 175-212, Chapman & Hall / CRC, London, UK, 2010.

SCIENTIFIC JOURNALS

47. Luo, M.; Wang, X.S.; Roth, B.L.; Golbraikh, A.; Tropsha, A. J. Chem. Inf. Model. 2014 Jan 10. [Epub ahead of print]

46. Golbraikh, A.; Muratov, E.; Fourches, D.; Tropsha, A. Data Set Modelability by QSAR. J. Chem. Inf. Model. 2014 Jan 8. [Epub ahead of print]

45. Low, Y.; Sedykh, A.; Fourches, D.; Golbraikh, A.; Whelan, M.; Rusyn, I.; Tropsha, A. Integrative chemical-biological read-across approach for chemical hazard classification. Chem. Res. Toxicol. 2013, 26,1199-1208.

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43. Martin, T.M.; Harten, P.; Young, D.M.; Muratov, E.N.; **Golbraikh, A.;** Zhu, H.; Tropsha, A. Does rational selection of training and test sets improve the outcome of QSAR modeling? *J. Chem. Inf.*

Model. **2012,** *52,* 2570-2578.

42. Bagheri, M.; Bagheri, M.; Gandomi, A.H.; **Golbraikh, A.** Simple yet accurate prediction method for sublimation enthalpies of organic contaminants using their molecular structure. *Thermochimica Acta* **2012**, *543,* 96-106.

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40. Bagheri, M,; **Golbraikh, A**. Rank-based ant system method for non-linear QSPR analysis: QSPR studies of the solubility parameter. *SAR QSAR Environ. Res.* **2012**, 23, 59-86.

39. Tropsha, A.; **Golbraikh, A.**; Won-Jea, C. Development of kNN QSAR Models for 3-Arylisoquinoline Antitumor Agents, *Bulletin of the Korean Chemical Society* **2011**, *32*, 2397-2404.

38. Hajjo, R.; Grulke, C.M.; **Golbraikh, A**.; Setola, V.; Huang, X.P.; Roth, B.L.; Tropsha, A. Development, validation, and use of quantitative structure-activity relationship models of 5-hydroxytryptamine (2B) receptor ligands to identify novel receptor binders and putative valvulopathic compounds among common drugs. *J. Med. Chem.* **2010,** *53*, 7573-86.

37. Zhu, H.; Ye, L.; Richard, A.; **Golbraikh, A.**; Wright, F.A.; Rusyn, I.; Tropsha, A. A Novel Two-step Hierarchical Quantitative Structure Activity Relationship Modeling Workflow for Predicting Acute Toxicity of Chemicals in Rodents. *Environ. Health Perspect.* **2009**, *117*, 1257-1264.

36. Zhang, L.; Zhu, H.; Oprea, T.I.; **Golbraikh, A.**; Tropsha, A. QSAR Modeling of the Blood-Brain Barrier Permeability for Diverse Organic Compounds. *Pharm. Res.* **2008,** *25,* 1902-1914.

35. Wang, X.S.; Tang, H.; **Golbraikh, A.**; Tropsha A. Combinatorial QSAR Modeling of Specificity and Subtype Selectivity of Ligands Binding to Serotonin Receptors 5HT1E and 5HT1F. *J. Chem. Inf. Model.* **2008,** *48,* 997-1013.

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33. Tropsha, A.; **Golbraikh, A.** Predictive QSAR modeling workflow, model applicability domains, and virtual screening. *Curr Pharm Des.* **2007**, 13, 3494-3504. Review.

32. Zhang, S.; **Golbraikh, A.**; Oloff, S.; Kohn, H.; Tropsha, A. A novel automated lazy learning QSAR (ALL-QSAR) approach: method development, applications, and virtual screening of chemical databases using validated ALL-QSAR models. *J Chem Inf Model.* **2006**, *46,* 1984-1995.

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16. **Golbraikh, A.;** Bonchev, D.; Xiao, Y.-D.; Tropsha, A. Novel Chiral Topological Descriptors and Their Application to QSAR. In: Rational Approaches to Drug Design. Proceedings of the 13th European Symposium on Quantitative Structure-Activity Relationships. 27 Aug – 1 Sept, 2000. Prous Science, **2001**, 219-223.

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14. **Golbraikh, A.** Molecular Dataset Diversity Indices and Their Applications to QSAR Analysis and Comparison of Chemical Databases. *J. Chem. Inf. Comput. Sci.* **2000**, 40, 414 – 425**.**

13. **Golbraikh, A.;** Bernard, P.; Chretien, J.R. Validation of protein-based alignment in 3D quantitative structure-activity relationships with CoMFA models. *Eur. J. Med. Chem.* **2000**, 35, 123 – 136.

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