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Computational scientist with 10 years of experience in designing & implementing computational infrastructures and the development of novel algorithms for life sciences data with a focus on pre-clinical small molecule drug discovery. My track record is evidenced by multiple deployed systems and more than 100 publications in peer reviewed journals. I have co-written multiple federally funded grants worth more than $2M. In addition I have extensive experience in public speaking, with more than 30 invited talks, as well as teaching workshops and classes at the graduate & undergraduate levels.

My goal is to impact therapeutic development by designing scalable computational methodologies that integrate heterogenous data types from multiple biological scales, to generate a global picture of the effects of small molecules in biological systems. I am particularly interested in linking chemical structure information to molecular, bibliographic genomic and clinical covariates to enable the study of polypharmacology and repurposing.

Professional Experience

01/01/2017 – ...	• Editor in Chief, *J. Cheminformatics*
07/01/2009 – ...	• Informatics Scientist, National Center for Advancing Translational Science, NIH
07/01/2009 – ...	• Adjunct Professor, School of Informatics, Indiana University
08/01/2007 – 06/31/2009	• Visiting Assistant Professor, School of Informatics, Indiana University
08/01/2006 – 07/30/2007	• Post-doctoral scholar working with Prof. D. Wild at Indiana University
08/01/2005 – 07/30/2006	• Post-doctoral scholar working with Prof. P. C. Jurs, Pennsylvania State University

Education

07/01/2001 – 07/30/2005	• Ph.D. (Chemistry), Department of Chemistry, The Pennsylvania State University.
05/01/1999 – 06/30/2001	• M.Sc. (Chemistry), Indian Institute of Technology, Kharagpur, India.
08/01/1995 – 07/30/1998	• B.Sc. (Chemistry), Presidency College, Calcutta, India.

Leadership & Mentoring

- Led the development and writing of the NCATS portion of two major grant applications (BARD and IDG Pharos) worth more than $2M
- Led the development of the complete informatics and analytic infrastructure underlying two key NCATS initiatives - the Trans NIH-RNAi Screening Facility & the NCATS Combination Screening Platform
- Developed and taught workshops on R for biologists at NCATS and EBI (Hinxton, UK) and involved in scientific mentoring of interns within the Informatics group
- Chair (2012) and Vice Chair (2011), ACS Division of Chemical Information
- Program Chair (2009-2010) and Asst. Program Chair (2007-2009), ACS Division of Chemical Information

Leadership & Mentoring (continued)

- Co-founder of the Blue Obelisk group, to promote Open Data, Open Source and Open Standards within chemistry. See Guha et al, 2006 & O'Boyle et al, 2011.

- Member of the editorial boards of Chemistry Central Journal, Current Computer Aided Drug Design, Journal of Cheminformatics and Synergy

- Organizer or co-organizer for multiple symposia at ACS National Meetings including *Scripting & Programming* (Fall 2009), *Systems Chemical Biology: Integrating Chemistry and Biology for Network Models* (Fall 2008) and *Cheminformatics Techniques in Bioinformatics* (Fall 2007)

Research & Development Experience

2009 – ...

- My duties at NCATS have ranged from infrastructure development for major center-wide initiatives as a well project specific algorithm development. Much of work has been collaborative and has required me to identify optimal solutions and achieve consensus amongst a variety of stakeholders.

  I led the development of the NCATS portions of Pharos, a user interface to the Knowledge Management Center of the Illuminating the Druggable Genome project and the BioAssay Research Database (BARD), a next generation chemical biology database. In both cases, I laid out the roadmap and designed the high level architecture of the systems and was responsible for maintaining the development schedule and interactions with our external collaborators.

  I have been responsible for the entire data management, visualization & analysis pipeline for the NCATS high throughput combination screening platform. Prior to this I developed the informatics infrastructure for the Trans-NIH RNAi Screening facility. have been instrumental in providing informatics support for high content screening projects, ranging from image analysis to informatics pipelines for the vendor integration, image storage and management and data mining methods.

  In parallel with infrastructure development, I have worked on a variety of more focused, problem specific areas. These include support for chemical probe development projects, including cherry picks, lead optimization and general cheminformatics analysis. Biologies covered include infectious disease, neurodegeneration and cancers.

  Recently I have been exploring approaches to mine large scale combination screening datasets. These include network models that allow one gain insight from large all-pair combination datasets and a novel similarity kernel that allows us to compare cell lines in "combination space". I also have ongoing efforts to develop and refine methods for the analysis of small molecule datasets from a variety of viewpoints - structure-activity landscapes, polypharmacology & promiscuity and scaffold based analyses that allow efficient summarization of large chemical datasets.

2007 – 2009

- Extended work on density of chemical space by using the R-NN method applied to compound selection in combinatorial libraries. I continued working on methods for handling large chemical datasets, including predictive modeling of HTS cytotoxicity data, virtual screening and QSAR modeling of large combinatorial libraries for anti-malarial activity and implentation of a fast 3D searching and pharmacophore matching in very large compound databases. During this period, I exmained methods to characterize activity landscapes and proposed approaches to explore promiscity and polypharmacology in PubChem bioassays using network models.

Research & Development Experience (continued)

2005 – 2007
- Implemented web service infrastructure to deploy integrated statistical and cheminformatics environments. Developed algorithm development for feature selection, analysis of large chemical spaces with applications to diversity analysis and clustering. Collaborated with Procter & Gamble to implement automated QSAR pipelines

Awards

2016 • NIH Directors Award (Malaria Combination Screening)
2015 • NIH Directors Award (Ebola Drug Repurposing)
2015 • Corwin-Hansch Award
2013 • NIH Directors Award (Malaria Screening)
2012 • Kelly Distinguished Performance Award
2011 • NIH Directors Award (Trans-NIH RNAi Screening)
2010 • Kelly Distinguished Performance Award
2007 • Jacques-Emile Dubois Grant Pennsylvania State University.

Computing & Data Science Experience

Languages
- Extensive experience with Java, Python, C and Unix shell scripting. Familiar with C++, Fortran and Lisp.
- Extensive experience with R for modeling and algorithm prototyping. Published and maintain packages that incorporate cheminformatics within R, handle molecular fingerprint data and interface R to the PubChem & ChEMBL bioassay and compound collections. Extended support for PMML in R

Platforms
- 10 years experience in developing J2EE based REST API's and clients using industry standard technology stacks. Experienced user of the OpenEye & ChemAxon toolkits, familiar with Pipeline Pilot, KNIME.

Databases
- Extensive experience with traditional RDBMS (Oracle, MySQL and PostgreSQL) and no-SQL databases (MongoDB), as well as integration of chemistry with databases

Memberships

- Member of the editorial boards of *Chemistry Central Journal*, *J. Cheminformatics* and *Curr. Drug Discov. Tech.*
- Member of the Scientific Advisory Board for the International Conference on Chemical Structures
- Member of the American Chemical Society

Publications

109. • Kalantat-Motamedi, Y.; Eastman, R.T.; **Guha, R.**; Bender, A.; "A systematic and prospectively validated approach for identifying synergistic drug combinations against malaria", *Malaria J.*, **submitted**, ,

108. • Calabrese, D.R.; Zlotkowski, K.; Alden, S.; Hewitt, W.M.; Connelly, C.M.; Wilson, R.M.; Gaikwad, S.; Chen, L.; **Guha, R.**; Thomas, C.J.; Mock, B.; Schneekloth, J.S.; "Small Molecule Microarray Profiling Reveals FDA Approved Drugs that Target the KRAS G-Quadruplex", *Angewandte Chemie*, **submitted**, ,

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105. • Oprea, T.I.; Bologa, C.G.; Brunak, S.; Campbell, A.; Gan, G.N.; Gaulton, A.; Gomez, S.M.; **Guha, R.**; Hersey, A.; Holmes, J.; Jadhav, A.; Jensen, L.J.; Johnson, G.L.; Karlson, A.; Leach, A.R.; Ma'ayan, A.; Malovannaya, A.; Mani, S.; Mathias, S.L.; McManus, M.T.; Meehan, T.F.; Mering, C.V.; Nguyen, D.; Overington, J.P.; Papadatos, G.; Qin, J.; Reich, C.; Schürer, S.C.; Simeonov, A.; Sklar, L.A.; Southall, N.; Tomita, S.; Tudose, I.; Ursu, O.; Vidović, D.; Waller, A.; Yang, J.J.; Zahoranszky-Köhalmi, G.; "Unexplored Therapeutic Opportunities in the Human Genome", **2017**, submitted

104. • McKinnon, T.; Venier, R.; Yohe, M.; Sindiri, S.; Gryder, B.; F., J.; Kabaroff, L.; Dickson, B.; Schleicher, K.; Chouinard-Pelletier, G.; Menezes, S.; Gupta, A.; Zhang, X.; **Guha, R.**; Ferrer, M.; Thomas, C.; Wei, Y.; Davani, D.; Guidos, C.; Khan, J.; Gladdy, R.; "PI3K/mTOR inhibition as a therapeutic strategy in FGFR4-driven rhabdomyosarcoma", *J. Clin. Invest.*, **2017**, submitted

103. • Mason, D.J.; Eastman, R.T.; **Guha, R.**; Lewis, R.P.I.; Stott, I.P.; Bender, A.; "The prediction of synergistic antimalarial drugs based upon known compound structure", **2017**, submitted

102. • Jansson, K.; Tucker, J.; Stahl, L.; Simmons, J.; Fuller, C.; Beshiri, M.; Agarwal, S.; Fang, L.; Hynes, P.; Alilin, A.; Cawley, J.; Lake, R.; Tran, C.; Tice, C.; Yin, J.; Zhang, X.; **Guha, R.**; Hoover, S.; Simpson, R.; Nguyen, H.; Corey, E.; Thomas, C.; Proia, D.; Kelly, K.; "High-throughput screen identifies HSP90 inhibitor efficacy across clinically-representative organoid models of advanced prostate cancer", *Clin. Cancer. Res*, **2017**, submitted

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100. • Feliz-Mosquea, Y.; Christensen, A.; Cook, K.; Schwartz, A.; Chen, Q.R.; Griner-Mathews, L.; **Guha, R.**; Thomas, C.; Ferrer, M.; Merino, M.J.; Roberts, D.; Pantoja, D.S; "Combination of anthracyclines and anti-CD47 therapy inhibit invasive breast cancer growth while preventing cardiac toxicity by regulation of autophagy", **2017**, submitted

99. • Zdrazil, B.; **Guha, R.**; "The rise and fall of a scaffold: A trend analysis of scaffolds in the medicinal chemistry literature", *J. Med. Chem.*, **2017**, in press

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96. • **Guha, R.**; Willighagen, E.L.; "Helping to improve the practice of cheminformatics", *J. Cheminf.*, **2017**, *9*,

95. • Lin, Y.; Mehta, S.; McGinty, H.K.; Turner, J.P.; Vidovic, D.; Forlin, M.; Koleti, A.; Nguyen, D.-T.; Jensen, L.J.; **Guha, R.**; Mathias, S.; Ursu, O.; Stathias, V.; Duan, J.; Nabizadeh, N.; Chung, C.; Mader, C.; Visser, U.; Yang, J.Bologa.; Oprea, T.I.; Schürer, S.C.; "Drug Target Ontology to Classify and Integrate Drug Discovery Data", *J. Biomed. Semantics*, **2017**, *8*,

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93. • Nguyen, D.-T.; Mathias, S.; Bologa, C.; Brunak, S.; Fernandez, N.; Gaulton, A.; Hersey, A.; Holmes, J.; Jensen, L.J.; Karlsson, A.; Lu, G.; Mayan, A.; Mandava, G.; Mani, S.; Mehta, S.; Overington, J.P.; Patel, J.; Rouillard, A.D.; Schurer, S.; Sheils, T.; Simeonov, A.; Sklar, L.; Southall, N.; Ursu, O.; Vidovic, D.; Waller, A.; J., Y.; Jadhav, A.; Oprea, T.I.; **Guha, R.**; "Pharos: Collating Protein Information to Shed Light on the Druggable Genome", *Nucl. Acids Res.*, **2017**, *45*, D995–D1002

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89. • Iniguez, A.B.; Alexe, G.; Wang, E.J.; Roti, G.; Patel, S.; Chen, L.; Kitara, S.; Conway, A.; Stolte, B.; Bandopadhayay, P.; Goodale, A.; Hall, M.; **Guha, R.**; Cheff, D.; Davis, M.; Qi, J.; Beroukhim, R.; Piccioni, F.; Johannessen, C.; Stegmaier, K.; "Enhancer remodeling promotes resistance to epigenetic-targeted therapy and engenders tumor cell vulnerabilities", *submitted*, **2017**, ,

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87. • Serra-Musach, J.; Mateo, F.; Capdevila-Busquets, E.; Zhang, X.; **Guha, R.**; Thomas, C.; Gruseo, J.; Ruiz de Garibay, G.; Villaneuva, A.; Gustafsson, M.; Benson, M.; Jaeger, S.; Heyn, H.; Vizoso, M.; Perez, H.; Cordero, A.; Gonzalez-Suarez, E.; Esteller, M.; Moreno-Bueno, G.; Lazaro, C.; Serra, V.; Arribas, J.; Ferrer, M.; Aloy, P.; Pujana, M.A.; "Cancer network activity associated with therapeutic response and synergism", *Genome Medicine*, **2016**, *8*, 1–12

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85. • Anantpadma, M.; Kouznetsova, J.; Wang, H.; Huang, R.; **Guha, R.**; Lindstrom, A.; Shtanko, O.; Simeonov, A.; Maloney, D.J.; Maury, W.; LaCount, D.; Jadhav, A.; Davey, R.; "Large Scale Screening and Identification of Novel Ebolavirus and Marburgvirus Entry Inhibitors", *Antimicrobial Agents and Chemotherapy*, **2016**, *60*, 4471–4481

84. • Chen, L.; Wilson, K.; Goldlust, I.S.; Mott, B.T.; Eastman, R.T.; Davis, M.I.; Zhang, X.; McKnight, C.; Klumpp-Thomas, C.; Shinn, P.; Simmons, J.; Gormally, M.; Michael, S.; Thomas, C.J.; Ferrer, M.; **Guha, R.**; "mQC: A Heuristic Quality-Control Metric for High-Throughput Drug Combination Screening", *Sci. Rep.*, **2016**, *6*, 1

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81. • Baranello, L.; Wojtowicz, D.; Kouzine, F.; Cui, K.; Chan-Salis, K.Y.; Devaiah, B.; Wilson, K.; **Guha, R.**; Thomas, C.; Singer, D.; Pommier, Y.; Pugh, B.F.; Przytyka, T.M.; Lewis, B.A.; Zhao, K.; Levens, D.; "RNA Polymerase II Regulates Topoisomerase 1 Activity to Favor Efficient Transcription", *Cell*, **2016**, *165*, 357–371

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5. • **Guha, R.**; Jurs, P.C.; "Determining the Validity of a QSAR Model–A Classification Approach", *J. Chem. Inf. Model.*, **2005**, *45*, 65–73

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Books and Book Chapters

- **Guha, R.**; Das, S.; "Exploring the Role of Small Molecules in Biological Systems Using Network Approaches" in '*Computational Network Analysis with R*', Eds. Dehmer, M.; Shi, Y.; Emmert-Streib, F.; Wiley-VCH Verlag GmbH; **2016**; pp. 151–172

- **Guha, R.**; "On Exploring Structure Activity Relationships" in '*In silico Models for Drug Discovery*', Ed. Kortegere, S.; Humana Press; **2013**; pp. 81–94

- **Guha, R.**; Bender, A. (Eds.); *Computational Approaches in Cheminformatics and Bioinformatics*; John Wiley & Sons, New York.; **2012**

- **Guha, R.**; "Collaborative Cheminformatics Applications' in '*Collaborative Computational Technologies for Biomedical Research*, Eds. Eakins, S., Hupcey, M.A.Z., Williams, A.J.;Wiley, New York; **2011**; pp. 399–422

- **Guha, R.**; "The Ups and Downs of Structure-Activity Landscapes' in '*Cheminformatics and Computational Chemical Biology*, Eds. Bajorath, J.; Springer, Berlin; **2011**; pp. 101–107

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- Ghosh, D.; **Guha, R.**; "A Risk Factor Analysis of West Nile Virus: Extraction of Relationships from a Neural Network Model" in *Advances in Social Computing, Proc. 3rd Intl. Conf. Social Computing, Behavioral Modeling and Prediction, SBP 2010*; Eds. Chai, S.-K.; Salerno, J.J.; Mabry, P.L.; Springer, Berlin; **2010**

Books and Book Chapters (continued)

- Bradley, J.C.; **Guha, R.**; Lang, A.; Lindenbaum, P.; Neylon, C.; Williams, A.; Willighagen, E.; "Beautifying data in the real world" in *Beautiful Data - The Stories Behind Elegant Data Solutions*, Segaran, T.; Hammerbacher, J. (Eds.), O'Reilly and Associates, **2009**
- Fox, G.C.; **Guha, R.**; McMullen, D.F.; Mustacoglu, A.F.; Pierce, M.; Topcu, A.E.; Wild, D.J.; "Web 2.0 for Grids and e-Science" in *Proc. INGRID 2007 - Instrumenting the Grid*, **2008**

Invited Presentations

April 2017 • Talk titled *Pharos A Torch to Use in Your Journey In the Dark Genome* at the BD2K-LINCS Data Science Research Webinar Series.

October 2016 • Talk titled *Enhancing Prioritization & Discovery of Novel Combinations using an HTS Platform* at the 7th American Conference on Pharmacometrics, Bellevue, WA.

September 2016 • Talk titled *Expanding the Dimensionality of Screening: From Single Agent Libraries to a Combination Screening Platform* at Merck Laboratories, Boston, MA.

August 2016 • Talk titled *What can your library do for you?* at the ACS National Meeting, Philadelphia, PA.

September 2015 • *Exploring & Quantifying Compound Combinations in High Throughput Settings: Going Beyond 1D Metrics* at MipTec, Basel, Switzerland.

August 2015 • *Characterization of Chemical Libraries Using Scaffolds and Network Models* at the ACS National Meeting, Boston, MA.

August 2015 • *So I have an SD File . . . What do I do next?* at the ACS National Meeting, Boston, MA.

July 2015 • *Multidimensional descriptors, multidimensional responses: Computational challenges facing QSAR* at Gordon Research Conference, CADD, Mt Snow, VT.

February 2015 • *From Data to Action: Bridging Chemistry and Biology with Informatics at NCATS* at Georgetown University, Washington D.C.

June 2014 • *Exploring Combinations in High throughput Settings* at Novartis, Boston, MA.

March 2014 • *When the Whole is Better than the Sum – Analytics to Support High Throughput Combination Screening* at Advancing Computational Biology Symposium, Howard University, Washington D.C.

January 2014 • *Exploring Compound Combinations in High Throughput Settings: Going Beyond 1D Metrics* at SLAS, San Diego, CA.

December 2012 • *Data Driven Discovery in Chemistry and the Tools to Enable It* at CSIR, New Delhi, India.

December 2012 • *Predicting Biological Activity from Molecular Structure* at Presidency University, Kolkata, India.

September 2012 • *Cloudy, with a touch of cheminformatics* at the ChemAxon UGM, Boston, MA.

June 2012 • *Chemogenomics in the cloud. Is the sky the limit?* at Translational Bioinformatics in the Cloud, New Brunswick, NJ.

January 2012 • *Clustering and Classification to identify Hits in High Content RNAi Screens* at CHI High Content Analysis, San Francisco, CA.

September 2011 • *Smashing Molecules* at the Chemaxon UGM, San Diego, CA.

August 2011 • *Predicting Activity Cliffs - Can Machine Learning Handle Special Cases?* at the Joint Statistical Meeting, Miami Beach, FL.

May 2011 • *R & CDK: A Sturdy Platform in the Oceans of Chemical Data* at the Molecular Informatics Open Source Software, EBI, Hinxton, UK.

Invited Presentations (continued)

May 2011	• *Enabling Discoveries at High Throughput - Small molecule and RNAi HTS at the NCTT* at the ChEMBL group, EBI, Hinxton, UK.
May 2011	• *Enabling Discoveries at High Throughput - Small molecule and RNAi HTS at the NCTT* at Syngenta, Jealotts Hill, UK.
March 2011	• *Structure-Activity Relationships and Networks: A Generalized Approach to Exploring Structure-Activity Landscapes* at George Mason University, Fairfax, VA.
January 2011	• *High throughput, High Content Screening - Enhancing Throughput via Fragments and Automation* at Howard University, Washington D.C.
January 2011	• *High Throughput, High Content Screening - Automating the Pipeline* at CHI High Content Analysis, San Francisco, CA.
November 2010	• *Chemical IR Workshop* at TREC 2010, NIST, Gaithersburg, MD.
February 2010	• *Joining the Dots: Integrating High Throughput Small Molecule and RNAi Screens* at the CCMB Seminar Series, University of Michigan, Ann Arbor, MI.
January 2010	• *Prioritizing Scaffolds for Hit Selection in High Throughput Screening* at the 6th Indo-US Workshop on Mathematical Chemistry at Kolkata, India.
December 2009	• *Molecular Representation, Similarity and Search*, guest lecture at Drexel University.
August 2009	• *Crunching Molecules and Numbers in R* at the 238th ACS National Meeting at Washington, D.C.
April 2009	• *Open Source Cheminformatics: Tools and Data* at BioIT World, Boston, MA.
February 2009	• *Structure-Activity Relationships and Networks: A Generalized Approach to Exploring Structure-Activity Landscapes* at the Ontario Institute for Cancer Research, Toronto.
December 2008	• *Networks - More Than Just Pretty Pictures* at Vertex Pharmaceuticals, Cambridge, MA.
December 2008	• *A Network View of Structure-Activity Landscapes* at Drexel University, Philadelphia, PA.
December 2008	• *Networks - More Than Just Pretty Pictures* at the CGB Roundtable, Indiana University, Bloomington. IN.
October 2008	• *Structure-Activity Relationships and Networks: A Generalized Approach to Exploring Structure-Activity Landscapes* at the NIH Chemical Genomics Center, Rockville, MD.
August 2008	• *Defining and Using Structure Activity Landscapes* at Simulations Plus, Lancaster, CA.
June 2008	• *Numerical Characterization of Structure-Activity Relationships from a Medicinal Chemist's Point of View* at the 31st National Medicinal Chemistry Symposium, Pittsburgh, PA.
May 2008	• *Aspects of Model Quality & Applicability* at Pfizer Inc., Groton, CT.
March 2008	• *The Structure Activity Landscape Index: Visualization and Applications* at Eli Lilly & Co., Indianapolis, IN
January 2008	• *Characterizing and Utilizing Structure Activity Landscapes* at Abbott Laboratories, Chicago, IL.
August 2007	• *Characterizing the Density of Chemical Spaces and its Use in Outlier Analysis and Clustering* at the Novartis Institute for Biomedical Research, Cambridge, MA.

Invited Presentations (continued)

May 2007	• *The Development and Deployment of Predictive Toxicology Models* at the MLSCN Steering Committee Meeting, Philadelphia, PA.
February 2007	• *Making the Most of Predictive Models* at the Openeye Cup 8, Santa Fe, NM.
January 2007	• *The Role of the Neighborhood in QSAR Modeling and Cheminformatics* at the Dept. of Pharmaceutical Technology, Jadavpur University, Calcutta.
August 2006	• *Chemical Spaces: Modeling, Exploration & Understanding* at the CICC-MACE-Lilly Cheminformatics Workshop, Indianapolis, IN.
August 2006	• *Writing & Using Web Services* at the CICC-MACE-Lilly Cheminformatics Workshop, Indianapolis, IN.
April 2006	• *Navigating Molecular Haystacks: Tools & Applications* at the School of Informatics, Indiana University, Bloomington, IN.
March 2006	• *Computational Tools & Protocols For Drug Discovery* at the School of Pharmacy, University of Maryland, Baltimore, MD.
September 2005	• *Extending Validation and Providing Interpretability for QSAR Models* at the Jet Propulsion Laboratory, Pasadena, CA.
February 2005	• *The Validation and Interpretation of QSAR Models* at NCI, Frederick.