# Rajarshi Guha

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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 70 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, 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.

## Education

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

## Professional Experience

2009 – . . . **Research Scientist, National Center for Advancing Translational Science, NIH**

- Performed research into data mining & visualization methods for high dimensional chemical biology datasets, addressing aspects of polypharmacology, network models and structure-activity relationships
- Led the development of the BioAssay Research Database backend and REST API (http://bard.nih.gov), a next generation chemical biology database. Responsible for architectural design that allowed BARD to serve as an *extensible platform* for the deployment of predictive models & cheminformatics algorithms
- Implemented large scale infrastructure to support two major screening facilities - the NCATS combination screening platform & the Trans-NIH RNAi Screening Facility. Completely responsible for system design, data storage and management architecture and R-based analytic pipelines for data processing, visualization and predictive modeling of screening data
- Provided informatics support for high content screening, including development of informatics pipelines for the integration of vendor databases and data mining methods
- Provided key cheminformatics and computational chemistry support on various probe development projects across multiple therapeutic areas including infectious disease, oncology and neurodegenerative disease

## Professional Experience (continued)

2007 – 2009 **Visiting Assistant Professor, School of Informatics, Indiana University**

- Worked on a variety of methods to explore high dimensional chemical spaces using a density of space approach to recognize chemical structure clusters
- Implementation of a fast 3D searching and pharmacophore matching in very large compound databases
- Developed 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
- Taught 3-credit undergraduate and graduate seminar courses on cheminformatics and scientific programming

2005 – 2007 **Post-doctoral fellowships at Penn State University and Indiana University**

- Implemented web services and database infrastructure for large scale chemical datasets
- Integration of statistical environments and cheminformatics toolkits with a focus on deployment of predictive models and reproducibility of computational workflows
- Collaboration with Procter & Gamble to develop QSAR modeling pipeline

## Leadership & Mentoring

Led the development and writing of the NCATS portion of two major grant applications 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 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

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)

## Computing & Data Science Experience

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| Languages | Extensive experience with Java, Python, C and Unix shell scripting. Familiar with C++, Fortran and Lisp.<br><br>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 |

## Awards

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| 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. |

## Publications

91. Yohe, M.E.; Gryder, B.E.; Shern, J.F.; Chou, H.C.; Song, Y.K.; Liao, H.; Sindiri, S.; Mendoza, A.; Zhang, X.; **Guha, R.**; Haines, D.C.; Mathews-Griner, L.A.; Li, S.Q.; Ferrer, M.; Thomas, C.J.; Khan, J.; "Epigenetic Reprogramming of RAS-driven Rhabdomyosarcoma via MEK Inhibition", **2016**, submitted

90. Gryder, B.E.; Yohe, M.E.; Chou, H.C.; Zhang, X.; Song, Y.; Marques, J.; Schaefer, B.; Sen, N.; Patidar, R.; Wen, X.; Wei, J.; **Guha, R.**; Ferrer, M.; Lal-Nag, M.; Andresson, T.; Shern, J.F.; Zhao, K.; Thomas, C.J.; Khan, J.; "PAX3-FOXO1 establishes myogenic super enhancers and confers BET bromodomain vulnerability", **2016**, submitted

89. 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", **2016**, submitted

88. Mathews-Griner, L.A.; Zhang, X.; **Guha, R.**; McKnight, C.; Goldlust, I.S.; Lal, M.; Wilson, K.; Michael, S.; Titus, S.; Shinn, P.; Thomas, C.; Ferrer, M.; "Large Scale Pharmacological Profiling of 3D Tumor Models of Cancer Cells", *Cell Death & Disease*, **2016**, in press

87. 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.*, **2016**, in press

86. Lal-Nag, M.; McGee, L.; **Guha, R.**; Lengyel, E.; Kenny, H.A.; Ferrer, M.; "A high throughput screening model of the tumor microenvironment for ovarian cancer cell growth", *SLAS Discovery*, **2016**, in press

85. 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

84. 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

83. 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

82. Ceribelli, M.; Kelly, P.N.; Ganapathi, K.; Evbuomwan, M.; Stefania, P.; Shaffer, A.L.; Wright, G.; Xiao, W.; **Guha, R.**; Zhang, X.; Ferrer, M.; Hou, E.Z.; Jaffe, E.S.; Reizis, B.; Thomas, C.; Staudt, L.M.; "A druggable TCF4- and BRD4-dependent transcriptional network sustains malignancy in blastic plasmacytoid dendritic cell neoplasm", *Cancer Cell*, **2016**, *30*, 764–778

81. **Guha, R.**; Mathews-Griner, L.A.; Keller, J.; Fitzgerald, D.J.; Atignani, A.; Pastan, I.; Thomas, C.J.; Ferrer, M.; "Ranking Differential Drug Activities from Dose Response Synthetic Lethality Screens", *J. Biomol. Screen.*, **2016**, *21*, 942–955

80. 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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79. Van Voorhis, W.C. et al; "Open Source Drug Discovery with the Malaria Box Compound Collection for Neglected Diseases and Beyond", *PLoS Pathogens*, **2016**, *12*, e1005763

78. Jun, W.; Zhang, M.; Wilson, K.; Petrus, M.N.; Bamford, R.; Zhang, X.; **Guha, R.**; Ferrer, M.; Thomas, C.; Waldmann, T.A.; "Augmented efficacy of brentuximab vedotin combined with ruxolitinib and/or Navitoclax in a murine model of human Hodgkin's Lymphoma", *Proc. Nat. Acad. Sci.*, **2016**, *113*, 1624–1629

77. Cong, Y.; Dyall, J.; Hart, B.J.; DeWald, L.E.; Johnson, J.C.; Postnikova, E.; Zhou, H.; Gross, R.; Rojas, O.; Alexander, I.; Josleyn, N.; Zhang, T.; Michelotti, J.; Janosko, K.; Honko, A.; Holbrook, M.; Bennett, R.S.; Olinger, G.O.; Glass, P.J.; Thomas, C.; Mierzwa, T.; **Guha, R.**; Shinn, P.; Michael, S.; Klumpp-Thomas, K.; McKnight, C.; Hensley, L.; Jahrling, P.B.; "Evaluation of the Activity of Lamivudine and Zidovudine against Ebola Virus In Vitro and In Vivo", *PLoS One*, **2016**, *11*, e0166318

76. Antignani, A.; Mathews Griner, L.; **Guha, R.**; Simmon, N.; Pasetto, M.; Keller, J.; Huang, M.; Angelus, E.; Pastan, I.; Ferrer, M.; FitzGerald, D.; Thomas, C.; "Chemical Screens Identify Drugs that Enhance or Mitigate Cellular Responses to Antibody-toxin fusion proteins", *PLoS One*, **2016**, *11*, e0161415

75. Cheng, K.Chih-Chien.; Cao, S.; Raveh, A.; MacArthur, R.; Dranchak, P.; Chlipala, G.; Okoneski, M.T.; **Guha, R.**; Eastman, R.T.; Yuan, J.; Schultz, P.J.; Su, X.; Tamayo-Castillo, G.; Matainaho, T.; Clardy, J.; Sherman, D.H.; Inglese, J.; "Actinoramide A stereoisomer identified as potent anti-malarial from titration-based screening of marine natural product extracts", *J. Nat. Prod.*, **2015**, *78*, 2411–2422

74. Lewis, R.; **Guha, R.**; Korcsmaros, T.; Bender, A.; "Synergy Maps: Exploring compound combinations using network-based visualization", *J. Cheminf.*, **2015**, *7*,

73. Bogen, D.; Wei, J.S.; Azorsa, D.O.; Ormanoglu, P.; Buehler, E.; **Guha, R.**; Keller, J.M.; Mathews-Griner, L.A.; Ferrer, M.; Song, Y.K.; Liao, H.; Mendoza, A.; Gryder, B.E.; Sindri, S.; He, J.; Wen, X.; Zhang, S.; Shern, J.F.; Yohe, M.E.; Taschner-Mandl, S.; Shohet, J.M.; Thomas, C.J.; Martin, S.E.; Ambros, P.F.; Khan, J.; "Aurora B Kinase is a Potent and Selective Target in MYCN-driven Neuroblastoma", *Oncotarget*, **2015**, *6*, 35247–35262

72. Mott, B.T.; Eastman, R.T.; **Guha, R.**; Sherlach, K.S.; Siriwardana, A.; Shinn, P.; McKnight, C.; Michael, S.; Lacerda-Quieroz, N.; Patel, P.R.; Khine, P.; Sun, H.; Kasbeka, M.; Aghdam, N.; Fontaine, S.D.; Liu, D.; Mierzwa, T.; Mathews-Griner, L.A.; Ferrer, M.; Renslo, A.R.; Inglese, J.; Yuan, J.; Roepe, P.D.; Su, X.; Thomas, C.J.; "High-throughput matrix screening identifies synergistic and antagonistic antimalarial drug combinations", *Scientific Reports*, **2015**, *5*,

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70. Zhang, M.; Mathews-Griner, L.A.; Ju, W.; Duveau, D.; **Guha, R.**; Petrus, M.N.; Wen, B.; Maeda, M.; Shinn, P.; Ferrer, M.; Conlon, K.D.; Bamford, R.; Oshea, J.; Thomas, C.J.; Waldmann, T.A.; "Selective targeting of JAK/STAT signaling is potentiated by Bcl-xL blockade in IL-2-dependent adult T-cell leukemia", *Proc. Nat. Acad. Sci.*, **2015**, *112*, 12480–12485

69. Pasetto, M.; Antignani, A.; Ormanoglu, P.; Buehler, E.; **Guha, R.**; Pastan, I.; Fitzgerald, D.J.; "A whole genome RNAi screen highlights components of the ER/Golgi as a source of resistance to immunotoxin-mediated cytotoxicity", *Proc. Nat. Acad. Sci.*, **2015**, *112*, 1135–1142

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67. Hasson, S.; Fogel, A.I.; Wang, C.; MacArthur, R.; **Guha, R.**; Heman-Ackah, S.; Martin, S.E.; Youle, R.J.; Inglese, J.; "Chemogenomic profiling of endogenous PARK2 expression using a genome-edited coincidence reporter", *ACS Chem. Biol.*, **2015**, *10*, 1188–1197

66. Carver, J.; Dexheimer, T.S.; Hsu, D.; Weng, M.T.; **Guha, R.**; Jadhav, A.; Simeonov, A.; Luo, J.; "A high-throughput assay for small molecule destabilizers of the KRAS oncoprotein", *PLoS One*, **2014**, *9*, e103836

65. Inglese, J.; Dranchak, P.; Moran, P.; Jang, S.-W.; Cost, G.J.; Srinivasan, R.; **Guha, R.**; Martinez, N.; MacArthur, R.; Urnov, F.D.; Svaren, J.; "Genome editing-enabled HTS assays expand drug target pathways for Charcot-Marie-Tooth disease", *ACS Chem. Biol.*, **2014**, *9*, 2594–2602

64. Josse, R.; S.E., M.; **Guha, R.**; Ormanoglu, P.; Pfister, T.; Morris, J.; Doroshow, J.; Pommier, Y.; "ATR inhibitors VE-821 and VX-970 sensitize cancer cells to topoisomerase I inhibitors by disabling DNA replication initiation and fork elongation responses", *Cancer. Res.*, **2014**, *74*, 6968–6979

63. **Guha, R.**; Medina-Franco, J.L.; "On the Validity versus Utility of Activity Landscapes: Are All Activity Cliffs Statistically Significant?", *J. Cheminf.*, **2014**, *6*,

62. Howe, E.; de Souza, A.; Lahr, D.; Chatwin, S.; Montgomery, P.; Alexander, B.; Nguyen, D.-T.; Cruz, Y.; Stonish, D.; Walzer, G.; Jason, R.; Picard, S.; Liu, Z.; Rose, J.; Xiang, X.; Asiedu, J.; Durkin, D.; Levine, J.; Yang, J.; Schürer, S.; Braisted, J.; Southall, N.; Southern, M.; Chung, T.D.Y.; Brudz, S.; Tanega, C.; Schreiber, S.L.; Bittker, J.; **Guha, R.**; Clemons, P.; "BioAssay Research Database (BARD): Chemical biology and probe-development enabled by structured metadata and result types", *Nucl. Acids Res.*, **2014**, *43*, D1163–D1170

61. de Souza, A.; Bittker, J.; Lahr, D.; Brudz, S.; Chatwin, S.; Oprea, T.I.; Waller, A.; Yang, A.; Southall, N.; **Guha, R.**; Schurer, S.; Vempati, U.; Southern, M.R.; Dawson, E.S.; Clemons, P.A.; Chung, T.D.Y.; "An overview of the challenges in designing, integrating, and delivering BARD: A public chemical-biology resource and query portal for multiple organizations, locations, and disciplines", *J. Biomol. Screen.*, **2014**, *19*, 614–627

60. Ceribelli, M.; Priscilla, K.; Shaffer, A.L.; Wright, G.; Yang, Y.; Mathews-Griner, L.A.; **Guha, R.**; Shinn, P.; Keller, J.M.; Liu, D.; Patel, P.R.; Ferrer, M.; Joshi, S.; Nerle, S.; Sandy, P.; Normant, E.; Thomas, C.J.; Staudt, L.M.; "Blockade of oncogenic I$\kappa$B kinase activity in ABC DLBCL by small molecule BET protein inhibitors", *Proc. Natl. Acad. Sci.*, **2014**, *111*, 11365–11370

59. Mathews, L.; **Guha, R.**; Shinn, P.; Young, R.A.; Keller, J.; Liu, D.; Goldlust, I.S.; Yasgar, A.; McKnight, C.; Boxer, M.B.; Duveau, D.; Jiang, J.K.; Michael, S.; Mierzwa, T.; Huang, W.; Walsh, M.J.; Mott, B.T.; Patel, P.R.; Leister, W.; Maloney, D.J.; LeClair, C.A.; Rai, G.; Jadhav, A.; Peyser, B.D.; Austin, C.P.; Martin, S.; Simeonov, A.; Ferrer, M.; Staudt, L.M.; Thomas, C.J.; "High-throughput combinatorial screening identifies drugs that cooperate with Ibrutinib to kill ABC Diffuse Large B Cell Lymphoma cells", *Proc. Nat. Acad. Sci.*, **2014**, *111*, 2349–2354

58. Casson, L.; Howell, L.; Mathews, L.A.; Ferrer, M.; Southall, N.; **Guha, R.**; Keller, J.M.; Thomas, C.; Varmus, H.; Siskind, L.J.; Beverly, L.J.; "Inhibition of Ceramide Metabolism Sensitizes Human Leukemia Cells to Inhibition of BCL2-like Proteins", *PLoS One*, **2013**, *8*, e54525

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57. Dranchak, P.; MacArthur, R.; **Guha, R.**; Zuercher, W.J.; Drewry, D.H.; Auld, D.S.; Inglese, J.; "Profile of the GSK published protein kinase inhibitor set across ATP-dependent and-independent luciferases: Implications for reporter-gene assays", *PLoS One*, **2013**, *8*,

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## Publications (continued)

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27. Singh, N.; **Guha, R.**; Guilianotti, M.; Houghten, R.; Medina-Franco, J.L.; "Chemoinformatic Analysis of Drugs, Natural Products, Molecular Libraries Small Molecule Repository and Combinatorial Libraries", *J. Chem. Inf. Model.*, **2009**, *49*, 1010–1024

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23. **Guha, R.**; Van Drie, J.H.; "The Structure-Activity Landscape Index: Identifying and Quantifying Activity-Cliffs", *J. Chem. Inf. Model.*, **2008**, *48*, 646–658

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14. **Guha, R.**; "Chemical Informatics Functionality in R", *J. Stat. Soft.*, **2007**, *18*,

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## Publications (continued)

11. **Guha, R.**; Howard, M.T.; Hutchison, G.R.; Murray-Rust, P.; Rzepa, H.; Steinbeck, C.; Wegner, J.; Willighagen, E.L.; "The Blue Obelisk–Interoperability in Chemical Informatics.", *J. Chem. Inf. Model.*, **2006**, *46*, 991–998

10. Dutta, D.; **Guha, R.**; Jurs, P.C.; Chen, T.; "Scalable Partitioning and Exploration of Chemical Spaces using Geometric Hashing", *J. Chem. Inf. Model.*, **2006**, *46*, 321–333

9. **Guha, R.**; "Generating, Using and Visualizing Molecular Information in R", *R News*, **2006**, *3*, 28–33

8. Steinbeck, C.; Hoppe, C.; Kuhn, S.; Floris, M.; **Guha, R.**; Willighagen, E.L.; "Recent Developments of the Chemistry Development Kit (CDK) - An Open-Source Java Library for Chemo- and Bioinformatics", *Curr. Pharm. Des.*, **2006**, *12*, 2110–2120

7. **Guha, R.**; Stanton, D.T.; Jurs, P.C.; "Interpreting Computational Neural Network QSAR Models: A Detailed Interpretation of the Weights and Biases", *J. Chem. Inf. Model.*, **2005**, *45*, 1109–1121

6. **Guha, R.**; Jurs, P.C.; "Interpreting Computational Neural Network QSAR Models: A Measure of Descriptor Importance", *J. Chem. Inf. Model.*, **2005**, *45*, 800–806

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

4. **Guha, R.**; "Using R to Provide Statistical Functionality for QSAR Modeling in CDK to Provide Statistical Functionality for QSAR Modeling in CDK", *CDK News*, **2005**, *2*, 7–13

3. **Guha, R.**; Jurs, P.C.; "Development of Linear, Ensemble, and Nonlinear Models for the Prediction and Interpretation of the Biological Activity of a Set of PDGFR Inhibitors.", *J. Chem. Inf. Comput. Sci.*, **2004**, *44*, 2179–2189

2. **Guha, R.**; Jurs, P.C.; "The Development of QSAR Models To Predict and Interpret the Biological Activity of Artemisinin Analogues", *J. Chem. Inf. Comput. Sci.*, **2004**, *44*, 1440–1449

1. **Guha, R.**; Serra, J.R.; Jurs, P.C.; "Generation of QSAR Sets with a Self-Organizing Map.", *J. Mol. Graph. Model.*, **2004**, *23*, 1–14

## 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

## Books and Book Chapters (continued)

**Guha, R.**; "Open Source Cheminformatics Software & Database Technologies" in *A Handbook of Cheminformatics Algorithms*, pp. 343–362 , Faulon, J.-L.; Bender, A. (Eds.); Chapman & Hall/CRC, Boca Raton, FL;**2010**

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**

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

| | |
|---|---|
| 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. |
| 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. |

## Invited Presentations (continued)

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.

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.

## Invited Presentations (continued)

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.

## Contributed Presentations

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|---|---|
| August 2016 | Talk titled *Pharos: Shining Light on the Druggable Genome* at the ACS National Meeting, Philadelphia, PA. |
| September 2014 | Talk titled *Robots, Small Molecules and R* at Boston DataCon 2014. |
| April 2013 | Talk titled *The BioAssay Research Database* at the 245$^{th}$ ACS National Meeting at New Orleans, LA. |
| April 2013 | Talk titled *Characterization and visualization of compound combination responses in a high throughout setting* at the 245$^{th}$ ACS National Meeting at New Orleans, LA. |
| February 2012 | Talk titled *Genome-wide RNAi screen for lysosomal storage disorders* with A. Velayati, P. Tuzmen, S. Martin, E. Goldin and E. Sidranksy at the Lysosomal Disease Network World Symposium, San Diego, CA. |
| December 2010 | Poster titled *Development and Validation of a Cell-Based Assay to Identify Small Molecule Modulators of Tristetraprolin, a Critical Regulator of Inflammation* with Wang, H., Huang, R., Inglese, J., Austin, C.P., Horner, T.J., Kennington, B.A., Shockley, K.R., Tice, R., Johnson, R.L. and Blackshear, P. at the Tox21 Board Review Meeting, Chapel Hill, NC. |
| August 2010 | Talk titled *Data driven life sciences: The Pyramids meet the Tower of Babel* at the 240$^{th}$ ACS National Meeting at Boston, MA. |
| August 2010 | Talk titled *What makes a good structure activity landscape?* at the 240$^{th}$ ACS National Meeting at Boston, MA. |
| March 2010 | Talk titled *A Network Visualization of Structure Activity Landscapes* at the 239$^{th}$ ACS National Meeting at San Francisco, CA. |
| March 2010 | Talk titled *iTunes for chemistry and biology: Addressing usability in cheminformatics* (with D. Ngyuen, Y. Wang, N. Southall, R. Huang, A. Jadhav) at the 239$^{th}$ ACS National Meeting at San Francisco, CA. |
| March 2010 | Talk titled *Hit Triage in RNAi Screens - Makking Use of Interaction and Pathway Data to Enhance Hit Selection* at the GeneGO Users Group Meeting, Cambridge, MA. |
| February 2010 | *Joining the Dots: Integrating High Throughput Small Molecule and RNAi Screens* at the CCMB Seminar Series, University of Michigan, Ann Arbor, MI. |
| August 2009 | Talk titled *Crowdsourcing Non-Aqueous Solubility and Synthesis Using Open Notebook Science* (with J.-C. Bradley, K. Mirza, A. Lang and A. Williams) at 238$^{th}$ ACS National Meeting at Washington, D.C. |
| April 2009 | Poster titled *Automatic Functional Annotation of PubChem Bioassays* (with Julien Gobeill and Patrick Ruch) at the 3$^{rd}$ International Biocuration Conference, Berlin. |
| December 2008 | Talk titled *SQMD: Architecture for Scalable, Distributed Database System built on Virtual Private Servers* (with K. Kim and M. Pierce) at the 4$^{th}$ Intl. Conf on e-Science, Indianapolis, IN. |
| December 2008 | Talk titled *Open Drug Discovery in Malaria Research* (with J.-C. Bradley, P. Rosenthal, K. Mirza and J. Gut) at the 4$^{th}$ Intl. Conf on e-Science, Indianapolis, IN. |
| August 2008 | Talk titled *PubChem Bioassays as a Source of Polypharmacology* (with B. Chen and D. J.Wild) at the 236$^{th}$ ACS National Meeting at Philadelphia, PA. |

## Contributed Presentations (continued)

August 2008 — Talk titled *Processing Drug Discovery Raw Data Collaboratively and Openly Using Open Notebook Science* (with J.-C. Bradley and P. Rosenthal) at the 236th ACS National Meeting at Philadelphia, PA.

June 2008 — Talk titled *Characterizing the Structure Activity Landscape and Implications for Predictive Modeling and Molecular Representations* at the 5th Indo-US Workshop on Mathematical Chemistry at Duluth, MN.

April 2008 — Talk titled *Combining Global and Local Approaches to Model Domain Applicability* (with D. Stanton) at the 235th ACS National Meeting at New Orleans, LA.

April 2008 — Talk titled *I Don't Care Where My Data and Methods Are: A Web-Service Approach for Distributed Access to Methods, Data and Models* at the 235th ACS National Meeting at New Orleans, LA.

August 2007 — Talk titled *Random Forest Ensembles Applied to MLSCN Screening Data for Prediction and Feature Selection* (with S. Schürer) at the 234th ACS National Meeting at Boston, MA.

August 2007 — Poster titled *Using Semantic Information for Feature Selection* at the Gordon Research Conference on Computer Aided Drug Design at Tilton, NH.

May 2007 — Talk titled *Integrating R with the CDK: Enhanced Chemical Data Mining* at the Central Regional ACS Meeting, Covington, KY.

March 2007 — Talk titled *Spectral Clustering of Chemical Datasets* at the 233rd ACS National Meeting at Chicago, Il.

March 2007 — Talk titled *A Tiered Screen Protocol for the Discovery of Structurally Diverse HIV Integrase Inhibitors* at the 233rd ACS National Meeting at Chicago, Il.

September 2006 — Talk titled *Local Lazy Regression: Making Use of the Neighborhood to Improve QSAR Predictions* at the 232nd ACS National Meeting at San Fransisco, CA.

September 2006 — Poster titled *R-NN Curves: A Method for Diversity Analysis and Cluster Identification* at the 232nd ACS National Meeting at San Fransisco, CA.

March 2006 — Talk titled *Scalable Partitioning & Exploration of Chemical Spaces Using Geometric Hashing* at the 231st ACS National Meeting at Atlanta, GA.

February 2006 — Poster titled *A Tiered Screening Protocol for the Discovery of Structurally Diverse HIV Integrase Inhibitors* at the 2nd Annual Computation Day, Pennsylvania State University, University Park, PA.

August 2005 — Talk titled *Integrating R with the CDK for QSAR Modeling* at the 230th ACS National Meeting at Washington D.C.

August 2005 — Poster titled *Applications of Spectral Clustering to Chemical Datasets* at the 2005 Gordon Research Conference on Computer Aided Drug Design, Tilton, NH.

March 2005 — Talk titled *The Interpretation of Neural Network QSAR Models Using Weights & Biases* at the 229th ACS National Meeting at San Diego, CA.

August 2004 — Poster titled *How Well Can a QSAR Model Handle New Datasets?* at the 228th ACS National Meeting at Philadelphia, PA.

August 2003 — Poster titled *Generation of QSAR Sets With A Self Organizing Map* at the 226th ACS National Meeting at New York City, NY.