Curriculum Vitae: Balius, Trent E.

Trent E. Balius, Ph.D.
Computational Chemistry Scientist III

Contact Information.

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I. Education and Training. (reverse chronological order)

2014-2018, 2012-2013	University of California, San Francisco, San Francisco, CA; Postdoctoral Fellow/Scholar, Pharmaceutical Chemistry Mentor: Brian K. Shoichet
2013-2014	University of Toronto, Toronto, ON; Postdoctoral Fellow, Faculty of Pharmacy Mentor: Brian K. Shoichet
2006-2012	Stony Brook University, Stony Brook, NY; Ph.D. in Applied Math & Statistics / Computational Biology (GPA: 3.850) Mentor: Robert C Rizzo
2001-2006	University of Pittsburgh at Greensburg, Greensburg, PA; B.S. in Applied Mathematics, Summa Cum Laude (GPA: 3.852)
2001-2006	University of Pittsburgh, Pittsburgh, PA; Certificate in Western European Studies
2004-2005	University of Granada, Center of Modern Languages, Granada, Spain; Spanish Language and Culture, Study abroad

II. Fellowships. (reverse chronological order)

2014-2015	NIH National Research Service Award, Grant: F32GM108161, Docking the Proteome for New Ligands and Functional Associations.
2008-2012	NIH National Research Service Award, Grant: F31CA134201, Characterizing the Mechanism of Cancer-Causing and Resistance Mutations of EGFR.

III. Publications. (reverse chronological order)

21. Bender, B. J.; Gahbauer, S.; Luttens, A.; Lyu, J.; Webb, C. M.; Stein, R. M.; Fink, E. A.; **Balius, T. E.**; Carlsson, J.; Irwin, J. J.; Shoichet, B. K.; A Practical Guide to Large Scale Docking; *Nature Methods*, **2021**, doi:10.1038/s41596-021-00597-z, PMID: 34561691
20. Kamenik, A. S.; Singh, I.; Lak, P.; **Balius, T. E.**;*, Liedl, K. R.;*; Energy Penalties Enhance Flexible Receptor Docking in a Model Cavity, *Proc. Natl. Acad. Sci. U. S. A.*, **2021**, 118(36):e2106195118. doi: 10.1073/pnas.2106195118, PMID: 34475217

19. Van, Q. N.; Prakash, P.; Shrestha, R.; **Balius, T. E.**; Turbyville, T. J.; Stephen, A. G.; RAS nanoclusters: dynamic signaling platforms amenable to therapeutic intervention. Biomolecules, Review, **2021,** 11, 377. doi: 10.3390/biom11030377, PMID: 33802474, PMCID: PMC8000715

18. Stein, R. M.; Yang, Y.; **Balius, T.E.**; O'Meara, M. J.; Lyu, J.; Young, J.; Tang, K.; Shoichet, B. K.; Irwin, J. J. Property-unmatched decoys in docking benchmarks, JCIM, **2021**, 61, 2, 699–714. doi:10.1021/acs.jcim.0c00598, PMID: 33494610, PMCID: PMC7913603

17. Wan, X.; Yang, T.; Cuesta, A.; Pang, X.; **Balius, T. E.**; Irwin, J.; Shoichet, B. K.; Taunton, J. Discovery of Lysine-Targeted eIF4E Inhibitors through Covalent Docking. JACS, Communication, **2020**, 142, 11, 4960-4964. doi:10.1021/jacs.9b10377, PMID: 32105459, PMCID: PMC7136196

16. Tran T. H.; Alexander, P.; Dharmaiah, S.; Agamasu, C.; McCormick, F.; Nissley, D. V.; Esposito, D.; Simanshu, D. K.; Stephen, A. G.; **Balius, T. E.***; The small molecule BI-2852 induces a non-functional dimer of KRAS. *Proc. Natl. Acad. Sci. U. S. A.*, **2020,** 117 (7), 3363-3364. doi:10.1073/pnas.1918164117, PMID:32047043, PMCID: PMC7035607, (Letter to the Editor in response to Kessler *et al.*, **2019**).

    * corresponding author

15. Lyu, J.*; Wang, S.*; **Balius, T. E.***; Singh, I.*.; Levit, A.; Moroz, Y. S.; O'Meara, M. J.; Algaa, E.; Tolmachova K.; Tolmachev, A. A.; Shoichet, B. K.; Roth, B. L.; and Irwin, J. J.; Ultra-large library docking for discovering new chemotypes. *Nature* **2019**, 566, 224-229. doi:10.1038/s41586-019-0917-9, PMID: 30728502, PMCID: PMC6383769. * these authors contributed equally to this work.

14. Nnadi, C. I.; Jenkins, M. L.; Gentile, D. R.; Batemen, L. A.; Zaidman, D.; **Balius, T. E.**; Nomura, D. K.; Burke, J. E.; Shokat, K. M.; London, N; Novel K-Ras G12C Switch-II covalent binders destabilize Ras and accelerate nucleotide exchange. *J. Chem. Inf. Model.* **2018**, 58 (2), 464–471. doi:10.1021/acs.jcim.7b00399, PMID: 29320178, PMCID: PMC6179444

13. Allen, W. J.*; Fochtman, B.C.*; **Balius, T. E.;** Rizzo, R. C., Customizable de novo Design Strategies for DOCK: Application to HIVgp41 and Other Therapeutic Targets. *J. Comput. Chem.*. **2017**, 38 (30), 2641–2663. doi:10.1002/jcc.25052, PMID: 28940386, PMCID: PMC5659719.

12. **Balius, T. E.***; Fischer, M.*; Stein, R. M.; Adler, T. B.; Nguyen, C. N.; Cruz, A.; Gilson, M. K.; Kurtzman, T.; and Shoichet, B. K., Testing Inhomogeneous Solvation Theory in Structure-Based Ligand Discovery. *Proc. Natl. Acad. Sci. U. S. A.*, **2017**, 114 (33) E6839-E6846. doi:10.1073/pnas.1703287114, PMID: 28760952, PMCID: PMC5565424. * these authors contributed equally to this work.

11. Teng, Y.G; Berger, W.T.; Nesbitt, N.M.; Kumar, K.; **Balius, T.E.**;.Rizzo, R.C; Tonge, P.J.; Ojima, I.; Swaminathan, S.; Computer-Aided Identification, Synthesis, and Biological Evaluation of Novel inhibitors for Botulinum Neurotoxin Serotype A, *Bioorg. Med. Chem.*, **2015**, 23 (17), 5489-5495. doi:10.1016/j.bmc.2015.07.040, PMID: 26275678

10. Allen, W. J.*; **Balius, T. E.***; Mukherjee, S.; Brozell, S. R.; Moustakas, D. T.; Lang, P. T.; Case, D. A.; Kuntz, I. D.; Rizzo, R. C., DOCK 6: Impact of New Features and Current Docking Performance. *J. Comput. Chem.*, **2015**, 36 (15), 1132-1156, doi:10.1002/jcc.23905, PMID: 25914306, PMCID: PMC4469538. * these authors contributed equally to this work.

9. Merski M.*; Fischer, M.*; **Balius, T. E.***; Eidam, O, Shiochet, B. K.; Homologous ligands accommodated by discrete conformations of a buried cavity, *Proc. Natl. Acad. Sci. U. S. A.*, **2015** 112 (16), 5039-5044. doi:10.1073/pnas.1500806112, PMID: 25847998, PMCID: PMC4413287.

    * these authors contributed equally to this work.

    This paper was highlighted in science:

    Science, 2015, 348(6235), 645-646 doi:10.1126/science.348.6235.645-f

8. **Balius, T. E.***; Allen, W. J.*; Mukherjee, S.; Rizzo, R. C., Grid-Based Molecular Footprint Comparison Method for Docking and De Novo Design: Application to HIVgp41. J. Comput. Chem., **2013** 34 (14), 1226-1240, doi:10.1002/jcc.23245, PMID: 23436713, PMCID: PMC4016043.

    * these authors contributed equally to this work.

7. Berger, W. T.; Ralph, B. P.; Kaczocha, M.; Sun, J.; **Balius, T. E.**; Rizzo, R. C.; Haj-Dahmane, S.; Ojima, I.; Deutsch, D. G., Targeting Fatty Acid Binding Protein (FABP) Anandamide Transporters - A Novel Strategy

for Development of Anti-Inflammatory and Anti-Nociceptive Drugs. *PLOS One*, **2012**, 7 (12), doi:10.1371/journal.pone.0050968, PMID: 23236415, PMCID: PMC3517626.

6. Brozell, S. R.; Mukherjee, S.; **Balius, T. E.**; Roe, D. R.; Case, D. A.; Rizzo, R. C., Evaluation of DOCK 6 as a Pose Generation and Database Enrichment Tool. *J. Comput. Aided Mol. Des.*, **2012**, 26 (6), 749-773. doi:10.1007/s10822-012-9565-y, PMID: 22569593, PMCID: PMC3902891.
5. **Balius, T. E.**; Mukherjee, S.; Rizzo, R. C. Implementation and Evaluation of a Docking-Rescoring Method using Molecular Footprint Comparisons, *J. Comput. Chem.,* **2011**, *32* (10), 2273–2289. doi: 10.1002/jcc.21814, PMID: 21541962, PMCID: PMC3181325
4. Mukherjee, S.; **Balius, T. E.**; Rizzo, R. C. Docking Validation Resources: Protein Family and Ligand Flexibility Experiments. *J. Chem. Inf. Model.*, **2010**, *50* (11), 1986–2000. doi: 10.1021/ci1001982, PMID: 21033739, PMCID: PMC3058392.
3. McGillick, B. E.*; **Balius, T. E.***; Mukherjee, S.; Rizzo, R. C. Origins of Resistance to the HIVgp41 Viral Entry Inhibitor T20. *Biochemistry*, **2010**, *49* (17), 3575-3592. doi:10.1021/bi901915g, PMID: 20230061, PMCID: PMC2867330.

   * these authors contributed equally to this work.
2. Owonikoko T. K.; Ramalingam S. S.; Kanterewicz B.; **Balius T. E.**; Belani C. P.; Hershberger P. A. Vorinostat Increases Carboplatin and Paclitaxel Activity in Non-small Cell Lung Cancer Cells. *Int. J. Canc.,* **2010**, *126*, 743-755. doi:10.1002/ijc.24759, PMID: 19621389, PMCID: PMC2795066.
1. **Balius, T. E.**; Rizzo, R. C. Quantitative Prediction of Fold Resistance for Inhibitors of EGFR. *Biochemistry*, **2009**, *48* (35), 8435-8448. doi:10.1021/bi900729a, PMID: 19627157, PMCID: PMC2741091.
0. **Balius, T.E.** Application and Development of Computational Tools in Drug Discovery, Ph.D Dissertation, Stony Brook University, **2012.**, proquest link: http://gradworks.umi.com/35/21/3521714.html

In preparation.

NA

IV Patents.

1. Ojima, I.; Deutsch, D.; Kaczocha, M.; Berger, W. T.; Rizzo, R.; **Balius, T. E.** Alpha-and gamma-truxillic acid derivatives and pharmaceutical compositions thereof. United States Patent office; Publication date: 2015/7/2; Patent number: 20150183715; Application number: 14/413621

V. Honors and Awards. (reverse chronological order)

2017	2017 QBC Retreat Poster Award
2014	NIH National Research Service Award Fellow (F32)
2012	President's Award to Distinguished Doctoral Student
2010	Chemical Computing Group Excellence Award (COMP Division, ACS Spring)
2008	NIH National Research Service Award Fellow (F31)
2005	The National Dean's List
2004	Phi Kappa Phi Senior Honor Society
2003	United States Achievement Academy in Mathematics
2003	DaVinci Society, Juniors and seniors selected as exemplars of Pitt-Greensburg's Cardinal Points of academic excellence, leadership, service and international experience
2002	Phi Eta Sigma Freshman Honor Society
2001	University of Pittsburgh at Greensburg University Scholarship

VI. Research Activities.

Overview: During my career, I have developed and applied computational methods to impact drug discovery.

Current.

2008-pres. Dock Development: I participated in releases of DOCK v6.4-v6.8 (2010-2015) and DOCK v3.7.1(2015) and 3.7.2(2018), and help to develop docking test sets.

2013-pres. Studying flexibility in small-molecule protein binding.

2013-pres Receptor desolvation using GIST in the DOCK 3.7 scoring function

2016-pres. Large scale docking: Databases are growing ever bigger

2019-pres. RAS Comp Chem: we use computational chemistry methods to aid in discovering molecules that modulated RAS and RAS related proteins. Methods we deploy include molecular docking, molecular dynamics, free energy methods, and chemical informatics methods.

Past.

2006-2009 Quantitative prediction of fold resistance for inhibitors of EGFR

2009-2010 Origins of resistance of HIV-GP41 to peptide inhibitor T20, simulations in lipid membrane.

2012-2015 Large-scale docking: Alloying docking with chemical informatics, Similarity Ensemble Approach

2013-2015 Vitamin D3 receptor lead discovery

2017-2019 Ligand discovery against phosphatase PGAM5, associated in neural degenerative disorders

VII. Positions and Appointments. (reverse chronological order)

2019-pres Computational Chemistry Scientist III, Frederick National Laboratory for Cancer Research
2018-2019 Associate Specialist, University of California, San Francisco
2015-2018 Postdoctoral Scholar, University of California, San Francisco
2014-2015. Postdoctoral Fellow (NIH NRSA), University of California, San Francisco
2013-2014 Postdoctoral Fellow (NIH NRSA), University of Toronto
2012-2013 Postdoctoral Scholar, University of California, San Francisco
2008-2012 Research Fellow (NIH NRSA)
2008 Research Assistant
2007 Teaching Assistant: AMS 161, Stony Brook University
2007 Teaching Assistant: AMS 151, Stony Brook University
2003-2006 Pfizer Summer Student Scholarship, UPMC

Other Professional Memberships

2007-pres. American Chemical Society Member
2008-pres. DOCK Development Team
2011-pres. Society for Industrial and Applied Mathematics

VIII. Talks, Lectures, and Posters.

Talks

2008 **Balius T. E.**; Rizzo R. C., Computational binding models for ligands with EGFR: Characterizing the basis of resistance; AMS Graduate Student Conference. (Talk)

2008 **Balius, T. E.**, Inhibition and Conformational Shifts of EGFR Tyrosine Kinase Domain Using Molecular Dynamics; Stony Brook Joint Group Meetings in Computational Structural Biology (Talk)

2008 **Balius, T. E.**; Mukherjee, S., Using BlueGene to characterize protein ligand interactions with DOCK and NAMD; August 4th New York Blue Tutorial. (Talk)

2011 **Balius, T. E.;** Mukherjee, S.; Rizzo, R. C. Development and application of footprint similarity scoring as a docking and virtual screening tool; 241th American Chemical Society National Meeting & Exposition. (Talk)

2011 **Balius, T.E.**, Development and Application of a Rescoring Tool for Docking and Drug Discovery; Stony Brook Joint Group Meetings in Computational Structural Biology (Talk)

2012 **Balius, T.E.**, Application and Development of Computational Tools in Drug Discovery (Dissertation Defense Talk)

2015 **Balius T.E.**; Nguyen, CN; Fischer, M.; Cruz-Balberdy, A.; Kurtzman, T.; Gilson, M. K.; Shoichet, B. K.; Testing the effects of including receptor desolvation in docking calculations. 250th American Chemical Society National Meeting & Exposition. (Talk)

2016 **Balius, T.E.**; Accounting for receptor desolvation in molecular docking with testing on a model cavity. Mission Bay RIPS, research in progress seminars, UCSF.

2017 **Balius, T.E.**; Advances in molecular docking as a ligand discovery tool. QBI Happy Hour, 5-minute flash presentation, UCSF

2017 **Balius T.E.**; Fischer, M.; Stein, R. M.; Adler, T. B.; Nguyen, CN; Cruz-Balberdy, A.; Kurtzman, T.; Gilson, M. K.; Shoichet, B. K.; Testing a desolvation term in molecular docking on a model cavity. 253rd American Chemical Society National Meeting & Exposition. (Talk)

2017 **Balius, T.E.**; DOCK: where it is and where it is going. Webinar, SBGrid Consortium

2017 **Balius, T.E.**; Expanding Accessible Chemical Space for Ligand Discovery. Flash Talk, Quantitative Biology Consortium Retreat. (3-minute talk to advertise my poster)

2018 **Balius, T.E.**; Expanding Accessible Chemical Space for Ligand Discovery. Graduate Student and External Speaker Seminar Series. Department of BioMolecular Sciences. University of Mississippi (Job Talk)

2018 **Balius, T.E.**; Lyu, J; Wang, S.; Singh, I; Levit, A; O'Meara, M; McCorvy, J; Roth, B.L.; Irwin, J.J.; Shoichet, B.K.; Leveraging expanding purchasable chemical space for ligand discovery, 256th American Chemical Society National Meeting & Exposition. (Talk in Emerging Technologies in Computational Chemistry)

2018 **Balius, T.E.**; Fischer, M; Kurtzman, T.P.; Gilson, M.K.; Shoichet, B.K.; Incorporating solvation thermodynamic mapping into docking, 256th American Chemical Society National Meeting & Exposition. (Talk filled in for Tom Kurtzman)

2018 **Balius, T.E.**; Leveraging the rapid increase in accessible chemical space for ligand discovery. Seminar. NCI RAS Initiative, Frederick National Lab (Job Talk)

2018 **Balius, T.E.**; Leveraging rapidly expanding accessible chemical space for ligand discovery. Seminar. Chemistry Department, University of Waterloo (Job Talk)

2020 **Balius, T.E.**; Targeting interfaces of KRAS with itself and other proteins; 260th American Chemical Society National Meeting & Exposition. (Virtual Recorded Talk)

Lectures

2003 Guest Lecture: ENGR 0011 (Engineering Analysis) MATLAB® Tutorial. (University of Pittsburgh at Greensburg) (Dr. Llenas)

2007 Guest Lecture: AMS535 (Intro. Comp. Bio.) Introduction to Molecular Mechanics Poisson-Boltzmann / Generalized Born Surface Area Methods. (Stony Brook University) (Robert Rizzo)

2008 Guest Lecture: AMS535 (Intro. Comp. Bio.). MM-PBSA Validation Study. (Stony Brook University) (Robert Rizzo)

2009 Guest Lecture: AMS535 (Intro. Comp. Bio.) All-atom Molecular Dynamics Simulations of EGFR with Prediction of Inhibitors Fold Resistance. (Stony Brook University) (Robert Rizzo)

2010 Guest Lecture: AMS535 (Intro. Comp. Bio.) All-atom Molecular Mechanics. (Stony Brook University) (Robert Rizzo)

2010 Guest Lecture: AMS535 (Intro. Comp. Bio.) Enrichments and Rescoring. (Stony Brook University) (Robert Rizzo)

2011 Guest Lecture: AMS535 (Intro. Comp. Bio.) All-atom Molecular Mechanics. (Stony Brook University) (Robert Rizzo)

2011 Guest Lecture: AMS535 (Intro. Comp. Bio.) Enrichments and Rescoring. (Stony Brook University) (Robert Rizzo)

2019 Guest Lecture: MSB 530 (Bioinformatics) Computational Structural Methods for Ligand (Drug) Discovery. (Mount St. Mary's University) (Susan Martin)

2020 Guest Lecture: MSB 530 (Bioinformatics) Computational Structural Methods for Ligand (Drug) Discovery. (Mount St. Mary's University) (Susan Martin)

2021 Guest Lecture: MSB 530 (Bioinformatics) Computational Structural Methods for Ligand (Drug) Discovery. (Mount St. Mary's University) (Susan Martin)

2021 Guest Lecture: Honors Physics of Earth and Space Science (PEASS), Diversity in STEM from the prospective of a person with Dyslexia. (Governor Thomas Johnson Highschool) (Natalie St Fleur)

2021 Guest Lecture: Honors Chemistry, Using our understanding of molecular structures and interactions to impact drug discovery. (Governor Thomas Johnson Highschool) (Natalie St Fleur)

Posters

2005 **Balius T. E.**; Eiseman J. L.; Soni A. S.; Parker R. S., A MATLAB® Tool for Analyzing Two-drug Chemotherapy; 8th Annual Undergraduate Symposium in the Chemical and Biological Sciences at UMBC. (Poster)

2007 **Balius T. E.**; Rizzo R. C., Computational Binding Models for Ligands with EGFR: Characterizing the Basis of Resistance; 234th American Chemical Society National Meeting & Exposition. (Poster)

2007 **Balius T. E.**; Rizzo R. C., Computational Binding Models for Ligands with EGFR: Characterizing the Basis of Resistance; Chemistry Research Day, Stony Brook University. (Poster)

2008 **Balius T. E.**; Rizzo R. C., Computational Binding Models for Ligands with EGFR: Characterizing the Basis of Resistance. New York Structural biology Group, Winter Meeting, Weil Cornell Medical College. (Poster)

2008 **Balius, T. E.**; Rizzo R. C., Energetic and Structural Analysis of EGFR Inhibition Using Molecular Dynamic Simulations; ACS Mid-Atlantic Regional Meeting (MARM). (Poster)

2008 **Balius, T. E.**; Rizzo R. C., Energetic and Structural Analysis of EGFR Inhibition Using Molecular Dynamic Simulations; New York Structural biology Group, Summer Meeting, Cold Spring Harbor Laboratory (Poster)

2008 **Balius, T. E.**; Huang, Y.; Rizzo R. C., Energetic and Structural Analysis of EGFR Kinase Domain Inhibition Using Molecular Dynamics Simulations and Cross-Docking; 2nd ICB&DD Annual Symposium "Frontiers in Chemical Biology and Drug Discovery". Stony Brook University. (Poster)

2008 **Balius, T. E.**; Huang, Y.; Rizzo R. C., Energetic and Structural Analysis of EGFR Kinase Domain Inhibition Using Molecular Dynamics Simulations and Cross-Docking; Chemistry Research Day, Stony Brook University. (Poster)

2008 **Balius, T. E.**; Huang, Y.; McGillick, B.; Mukherjee, S.; Goyal, R.; Rizzo, R. C., Characterizing Binding of Peptide Inhibitors and Small molecules with HIVgp41 using Molecular Dynamics Simulations; 22nd Annual Meeting of Groups Studying the Structures of AIDS-related Systems and Their Application to targeted Drug Design. (Poster)

2009 Owonikoko, T. K.; Ramalingam S. S.; Kanterewicz, B.; **Balius T. E.**; Belani C. P.; Hershberger P. A., The histone deacetylase inhibitor, vorinostat, increases carboplatin and paclitaxel activity in non-small cell lung cancer cells; AACR Annual Meeting. (Poster)

2009 Mukherjee, S.; **Balius, T. E.**; Goyal, R.; Holden, P.; Huang, Y.; Ascher, K.; Rizzo, R. C. Optimization of DOCK for Virtual Screening; 23rd Annual Meeting of Groups Studying the Structures of AIDS-related Systems and Their Application to targeted Drug Design. (Poster)

2009 **Balius, T. E.**; Rizzo, R. C. Prediction of Fold Resistance for Inhibitors of EGFR using All-atom Molecular Dynamics Simulations; 238th American Chemical Society National Meeting & Exposition. (Poster)

2009 **Balius, T. E.**; Rizzo, R. C. Prediction of Fold Resistance for Inhibitors of EGFR using All-atom Molecular Dynamics Simulations; Inaugural Symposium for the Laufer Center for Computational Biology and Genome Sciences; Stony Brook University. (Poster)

2009 **Balius, T. E.**; Rizzo, R. C. Prediction of Fold Resistance for Inhibitors of EGFR using All-atom Molecular Dynamics Simulations; 3rd ICB&DD Annual Symposium “Frontiers in Chemical Biology and Drug Discovery"; Stony Brook University. (Poster)

2009 **Balius, T. E.**; Rizzo, R. C. Prediction of Fold Resistance for Inhibitors of EGFR using All-atom Molecular Dynamics Simulations; Chemistry Research Day, Stony Brook University. (Poster)

2010 **Balius, T. E.**; Rizzo, R. C. Computational prediction of fold resistance in EGFR drug resistance; 239th American Chemical Society National Meeting & Exposition. (Poster)

2010 Mukherjee, S.; **Balius, T. E.**; Rizzo, R. C. Pose Accuracy using DOCK: Database Construction and Protocol Evaluation; 24th Annual Meeting of Groups Studying the Structures of AIDS-related Systems and Their Application to targeted Drug Design. (Poster)

2010 **Balius, T. E.**; McGillick, B. E.; Mukherjee, S.; Holden, P.; Jiang, L.; Rizzo, R. C. Binding Characterization and Lead discovery Targeting HIVgp41; 24th Annual Meeting of Groups Studying the Structures of AIDS-related Systems and Their Application to targeted Drug Design. (Poster)

2010 **Balius, T. E.**; Mukherjee, S.;Rizzo, R. C. Molecular interaction footprints: A docking rescoring method; 240th American Chemical Society National Meeting & Exposition. (Poster)

2010 **Balius, T. E.**; Mukherjee, S.; Rizzo, R. C. Pose Accuracy using DOCK: Database Construction and Protocol evaluation; 240th American Chemical Society National Meeting & Exposition. (Poster)

2010 **Balius, T. E.**; Mukherjee, S.; Rizzo, R. C. Molecular Footprints as a Docking Rescoring Tool in Drug Discovery; 4th ICB&DD Annual Symposium “Drugs, Biologics, Devices, and the FDA"; Stony Brook University. (Poster)

2011 Mukherjee, S.; **Balius, T. E.**; Rizzo, R. C. Development of the SB2010 testset to evaluate docking; 241th American Chemical Society National Meeting & Exposition. (Poster)

2014 **Balius T.E.**; Fischer, M.; Cruz-Balberdy, A.; Kurtzman, T.; Gilson, M. K.; Shoichet, B. K.; Testing the importance of receptor desolvation for docking using a model system; 248th American Chemical Society National Meeting & Exposition. (Poster) – Presented in Sci-mix and comp division poster sections

2017 **Balius T.E.**; Developing and Applying Computational Approaches in Early-stage Drug Discovery; 254th American Chemical Society National Meeting & Exposition. (Poster) – Presented in Academic Employment Initiative

2017 Lyu, J.; Levit, A.; **Balius, T.E.**; Singh, I; McCorvy, J.; Wang, S; O’Meara, M; Shoichet, B.K.; Roth, B.L.; & Irwin, J.J.; Docking over 140 million available molecules for new biology, Quantitative Biology Consortium Retreat (received Poster Award)

2018 Lyu, J.*; Wang, S.*; **Balius, T. E.***; Singh, I.*.; Levit, A.; Moroz, Y. S.; O’Meara, M. J.; Algaa, E.; Tolmachova K.; Tolmachev, A. A.; Shoichet, B. K.; Roth, B. L.; and Irwin, J. J.; Leveraging rapidly expanding purchasable chemical space for ligand discovery. ASBMB, Special Symposia Series, The many faces of kinases and pseudokinases.

IX. Teaching experience.

2007 Teaching Assistant for Applied Calculus I (AMS151) and II (AMS161), I graded papers and held office hours.

2008-2012 I gave guest lectures in Introduction to Computational Structural Biology and Drug Design (AMS535); and I ran tutorials in Molecular Modeling of Biological Molecules (AMS536).

2017-2018 Provided support (office hours, attend hit picking parties) to first-year graduate students in the Chemical Biology Course (Chemistry 243) for the docking segment.

2018 I took the STEP-UP (Science Teaching Effectiveness Program for Upcoming Professors) Introduction to Pedagogy Course

2019 Guest lecture at Mount St. Mary's.

2020 Guest lecture at Mount St. Mary's over zoom.

2021 Guest lecture at Mount St. Mary's over zoom.

2021 Guest lecture to Honors Physics of Earth and Space Science Class at Governor Thomas Johnson High School

2021 Guest lecture to Honors Chemistry Class at Governor Thomas Johnson High School

X. Mentoring and Supervising.

supervising at the Frederick National Lab.

Dates	Name	Program or School	Role	Current Position
2020-pres.	Priyanka Prakash	CTRP, FNL	Computational Scientist II	

Mentoring at the Frederick National Lab.

Dates	Name	Program or School	Role	Current Position
2019-2019	Alyssa M Klein	SCRTA NIH Intern, Bioinformatics master's student at Hood College	Summer Intern advisor (8-week internship)	Bioinformatics Scientist (NIH/NCI Contractor) at Kelly
2019-2019	Muyan Zhoa	Biostatistics master's Student at Georgetown University	Summer Intern advisor (6 weeks)	NA
2021-2021	Dillon Chu	Bioinformatics Master's Program Student at Georgetown University	Summer Intern advisor (8-week internship)	NA

Mentoring during Postdoctoral Work.

Dates	Name	Program or School	Role	Current Position
2015 – 2019	Reed M. Stein	PSPG graduate student at UCSF	Rotation and Graduate Research mentor in Shoichet lab	Scientist, Denali Therapeutics

2015 – 2015	Nivedita Titus	High school LPS Richmond	Job Shadow, 4-day visit	
2015 – 2015	Jennifer Martinez	High school LPS Richmond	Job Shadow, 2-day visit	
2015 – 2015	Anna Sophia Kamenik	Visiting graduate student at UCSF	Research mentor (3 months) in Shoichet lab	Postdoctoral Researcher, ETH Zürich
2015 - 2019	Chimno Nnadi	MD/PhD student, CCB graduate program	Research mentor, she is in the Shokat Lab	Medical Student
2016 - 2018	Jainkun Lyu	Visiting graduate student at UCSF	Research mentor (2 years) in Shoichet lab	Postdoc at UCSF
2017 - 2019	Chase Webb	PSPG graduate student at UCSF	Rotation and Graduate Research mentor in Shoichet lab	NSF Predoctoral Fellow

Mentoring during Graduate Work.

Dates	Name	Program or School	Role	Current Position
2007-2008	Yulin Huang	Graduate program in Biochemistry at Stony Brook University	Rotation project mentor in the Rizzo Lab	
2008 – 2008	Chetan Raj Rupakheti	Visiting undergrad, Stony Brook University	Summer projects mentor in Rizzo Group	Postdoctoral Scholar at University of Chicago
2008-2009	Brian McGillick	Masters student in Biomedical engineering at SBU	Rotation project mentor in Rizzo lab	Resident Physician, University of Cincinnati
2009 – 2009	Kenneth B. Ascher	Undergraduate Math major at SBU	Undergraduate Research Mentor in Rizzo Group	NSF Postdoctoral Fellow, Massachusetts Institute of Technology
2010 – 2011	Jibril Ashiru-Balogun	Undergraduate	Undergraduate Research Mentor in Rizzo Group	
2010-2011	Lingling Jiang	Grauate Student in AMS at SBU	Rotation Project mentor in Rizzo Lab	Novo Nordisk

XI. Public Service.

Ad hoc Reviewer for the Following Journals:
2013 International Journal of Molecular Sciences (http://www.mdpi.com/journal/ijms/)
2014 Nature Communications (http://www.nature.com/ncomms/index.html)
2014 Journal of Chemical Information and Modeling (https://pubs.acs.org/journal/jcisd8)
2015 Journal of Computer Aided Molecular Design (http://www.springer.com/chemistry/physical+chemistry/journal/10822)
2015 Emerging Microbes & Infections (http://www.nature.com/emi/index.html)
2016 Journal of Medicinal Chemistry (http://pubs.acs.org/journal/jmcmar)
2018 PLOS ONE (http://journals.plos.org/plosone/)
2021 Nature Communications (http://www.nature.com/ncomms/index.html)

Grant reviewer.
2022 Canada Foundation for Innovation - peer review committee

Presider of ACS COMP section
253rd, 250th, 248th, and 241th American Chemical Society
Judge for Undergrad posters at COMP poster section for 253rd ACS.

DOCK activities.
2008-pres. Active on DOCK-fans mailing lists.
2013-pres. In charge of approving academic (and non-profit) DOCK license applications.
2021 Lead virtual DOCK developers meeting for 9 months

XII. Technical Skills.

Platforms: PC Linux, Windows 10
Languages and Environments: C++, C, Fortran90, shell-scripts, Python, HTML, MATLAB, CVS repository, SVN repository, GitHub
Modeling Software: Amber 14, NAMD, DOCK6.X, DOCK3.X; MOE, VMD, Chimera