Trent E. Balius, Ph.D.

Contact Information.

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Webpage:	http://www.docking.org/~tbalius

I. Education and Training.

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
2006-2012	Stony Brook University, Stony Brook, NY; Ph.D. in Applied Math & Statistics / Computational Biology (GPA: 3.850)
2013-2014	University of Toronto, Toronto, ON; Postdoctoral Fellow, Faculty of Pharmacy
2012-2013, 2014-pres	University of California, San Francisco, San Francisco, CA; Postdoctoral Scholar, Pharmaceutical Chemistry

II. Fellowships.

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

III. Honors and Awards.

2001	University of Pittsburgh at Greensburg University Scholarship
2002	Phi Eta Sigma Freshman Honor Society
2003	DaVinci Society
2003	United States Achievement Academy in Mathematics
2004	Phi Kappa Phi Senior Honor Society
2005	The National Dean's List
2008	NIH National Research Service Award Fellow (F31)
2010	Chemical Computing Group Excellence Award (COMP Division, ACS Spring)
2012	President's Award to Distinguished Doctoral Student
2014	NIH National Research Service Award Fellow (F32)
2017	2017 QBC Retreat Poster Award

IV. Research Activities.

2006-2009 Quantitative prediction of fold resistance for inhibitors of EGFR
- Assignment of parameter to small molecules
- Performed MD simulations with AMBER
- Free energy calculations (MM-GBSA)
- Footprint calculations
- Explicit Solvation analysis (highly populated waters)
- Gained valuable experience in scripting language
  - Shell scripts, Python, etc.

2009-2010 HIV-GP41 (Collaboration)
- Performed MD simulations with NAMD
- Experience running membrane simulations
- Interaction Matrices (similar to footprints)
- Error analysis (BASEM, and ACF)
- Radial Distribution functions

2008-pres. Dock Development (Collaboration)

Participated in releases of DOCK v6.4-v6.8 (2010-2015) and DOCK v3.7.beta2 (2015)
- Sampling improvements
- Scoring/Rescoring methods
  - Footprint Similarity Score (DOCK v6.5)
  - Grid-based Footprint Similarity Score (DOCK v6.6)
  - Multi receptor grid-based docking (DOCK 6 development)
  - Added GIST component to DOCK 3.7 scoring function
- Experience developing the source code
  - C++ and Fortain programming
  - Github and CVS repository skills
- Docking Testset Development

2012-pres. Large scale docking
- Automated Docking with DOCK Blaster Tool Chain
- Chemical informatics: Similarity Ensemble Approach (SEA)
- Databases are growing ever bigger

2013-2015 Vitamin D3 Receptor Lead Discovery.

2013-pres Receptor Desolvation using GIST in the DOCK 3.7 Scoring function.

V. Positions and Appointments.

2003-2006 Pfizer Summer Student Scholarship, UPMC
2007 Teaching Assistant: AMS 151, Stony Brook University
2007 Teaching Assistant: AMS 161, Stony Brook University
2008 Research Assistant
2008-2012 Research Fellow (NRSA)
2012-2013 Postdoctoral Scholar, University of California, San Francisco
2013-2014 Postdoctoral Fellow, University of Toronto
2014-pres. Postdoctoral Scholar, University of California, San Francisco

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

VI. Publications.

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.
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.
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.
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.
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
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.
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.
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.
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.
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.
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
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.

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.
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

VII 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

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)

Lectures

2003 Guest Lecture: ENGR 0011 (Engineering Analysis) MATLAB® Tutorial

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

2008 Guest Lecture: AMS535 (Intro. Comp. Bio.). MM-PBSA Validation Study.

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

2010 Guest Lecture: AMS535 (Intro. Comp. Bio.) All-atom Molecular Mechanics.

2010 Guest Lecture: AMS535 (Intro. Comp. Bio.) Enrichments and Rescoring.

2011 Guest Lecture: AMS535 (Intro. Comp. Bio.) All-atom Molecular Mechanics.

2011 Guest Lecture: AMS535 (Intro. Comp. Bio.) Enrichments and Rescoring.

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)

IX. Teaching experience.

2007 Teaching Assistant for AMS151 and AMS161, graded papers and held office hours.

2008-2012 Guest lectures in AMS535; and tutorials in AMS536.

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

X. Mentoring.

During Graduate Work.

2007-2012 Yulin Huang (Biochemistry Graduate student

2008 Chetan Raj Rupakheti (visiting undergrad)

2008-2010 Brian McGillick (Biomedical engineering MS)

2009 Kenneth Asher, undergraduate Math major at SBU

2009-2012 Patrick Holden, continuing educations, MS

2010 Brian Shea, undergraduate

2010-2011 Jibril Ashiru-Balogun, undergraduate

2010-2012 Lingling Jiang, AMS PhD

During Postdoctoral Work.

2014-2016 Thomas B Adler, Pharmaceutical Chemistry Postdoc.

2014-pres. Xiaobo Wan, Pharmaceutical Chemistry Postdoc.

2015 Nivedita Titus and Jennifer Martinez. High school students from Leadership Public School, Richmond. I mentored them for four-days. I planned activities to give them the experience of working at a research university.

2015-pres. Reed M. Stein, PSPG graduate student at UCSF.

2015 Anna Sophia Kamenik, Visiting graduate at UCSF (3 months)

2015-pres. Chimno Nnadi (MD/PhD student, CCB graduate program)

2016-pres. Jainkun Lyu, Visiting graduate student at UCSF (2 years)

2017 Chase Webb (PSPG graduate student, rotation student)

XI. Public Service.

Ad hoc Reviewer for the Following Journals:
International Journal of Molecular Sciences (http://www.mdpi.com/journal/ijms/)
Nature Communications (http://www.nature.com/ncomms/index.html)

Journal of Computer Aided Molecular Design
(http://www.springer.com/chemistry/physical+chemistry/journal/10822)
Emerging Microbes & Infections (http://www.nature.com/emi/index.html)
Journal of Medicinal Chemistry (http://pubs.acs.org/journal/jmcmar)
PLOS ONE (http://journals.plos.org/plosone/)

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.

XII. Technical Skills.

Platforms: PC Linux, Windows NT/2000
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