

BIOGRAPHICAL SKETCH

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NAME Trent E. Balius		POSITION TITLE Ph.D. Student	
eRA COMMONS USER NAME TBALIUS			
EDUCATION/TRAINING <i>(Begin with baccalaureate or other initial professional education, such as nursing, and include postdoctoral training.)</i>			
INSTITUTION AND LOCATION	DEGREE <i>(if applicable)</i>	YEAR(s)	FIELD OF STUDY
University of Pittsburgh at Greensburg, Greensburg, PA	B.S.	2001-2006	Applied Mathematics
University of Pittsburgh, Pittsburgh, PA	Certificate	2001-2006	Western European Studies
University of Granada, Center of Modern Languages, Granada, Spain		2004-2005	Spanish Language and Culture, Study abroad
Stony Brook University, Stony Brook, NY	Ph.D. student	2006-pres	Applied Math & Statistics / Computational Biology

A. Positions and Honors.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
2003-2006	Pfizer Summer Student Scholarship
2004	Phi Kappa Phi Senior Honor Society
2005	The National Dean's List
2006	B.S., Applied Mathematics, University of Pittsburgh at Greensburg, Summa Cum Laude
2008	NIH National Research Service Award Fellow
2010	Spring 2010 CCG Excellence Graduate Student Travel Award (COMP Division, ACS)

Other Professional Activities

2007	Teaching Assistant: AMS 151, Stony Brook University
2007	Teaching Assistant: AMS 161, Stony Brook University
2007-pres.	American Chemical Society Member
2008	Research Assistant
2008-pres.	Research Fellow (NRSA)

B. Presentations / Posters.

2003	Guest Lecture: ENGR 0011 (Engineering Analysis) MATLAB® Tutorial
2005	Balius T. E. ; Eiseman J. L.; Soni A. S.; Parker R. S., A MATLAB® Tool for Analyzing Two-drug Chemotherapy; 8 th 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; 234 th American Chemical Society National Meeting & Exposition. (Poster)
2007	Guest Lecture: AMS535 (Intro. Comp. Bio.). Introduction to Molecular Mechanics Poisson-Boltzmann / Generalized Born Surface Area Methods.
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; AMS Graduate Student Conference. (Presentation)
- 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)
- 2008 **Balius, T. E.**; Mukherjee, S., Using BlueGene to characterize protein ligand interactions with DOCK and NAMD; August 4th New York Blue Tutorial. (Presentation)
- 2008 Guest Lecture: AMS535 (Intro. Comp. Bio.). MM-PBSA Validation Study.
- 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.** and 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.** and 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.** and 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.** and Rizzo, R. C. Prediction of Fold Resistance for Inhibitors of EGFR using All-atom Molecular Dynamics Simulations; Chemistry Research Day, Stony Brook University. (Poster)
- 2009 Guest Lecture: AMS535 (Intro. Comp. Bio.). All-atom Molecular Dynamics Simulations of EGFR with Prediction of Inhibitors Fold Resistance.
- 2010 **Balius, T. E.** and 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)

Principal Investigator/Program Director (Last, First, Middle): Rizzo, Robert C.

- 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.** and Rizzo, R. C. Molecular interaction footprints: A docking rescoring method; 240th American Chemical Society National Meeting & Exposition. (Poster)
- 2010 **Balius, T. E.** and 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)
- 2010 Guest Lecture: AMS535 (Intro. Comp. Bio.). All-atom Molecular Mechanics.
- 2010 Guest Lecture: AMS535 (Intro. Comp. Bio.). Enrichments and Rescoring.
- 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 Mukherjee, S.; **Balius, T. E.**; Rizzo, R. C. Development of the SB2010 testset to evaluate docking; 241th American Chemical Society National Meeting & Exposition. (Poster)

C. 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](https://doi.org/10.1021/bi900729a) PMID: 19627157
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. *International Journal of Cancer* **2010**, *126*, 743-755 [doi:10.1002/ijc.24759](https://doi.org/10.1002/ijc.24759) PMID: 19621389
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](https://doi.org/10.1021/bi901915g)
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), pp 1986–2000 [doi: 10.1021/ci1001982](https://doi.org/10.1021/ci1001982)
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](https://doi.org/10.1002/jcc.21814) PMID: 21541962
6. **Balius, T. E.**; Bai, L; Clausen, D. M.; Eiseman, J. L.; Soni, A. S; Parker, R. S., A Mathematical Tool for Analyzing Combination Cancer Treatment in vitro and in vivo (*submitted jan. 2011 to Comput. Biol. Med.*)

D. Technical Skills.

Platforms: PC Linux, Windows NT/2000

Languages and Environments: C, C++, shell-scripts, Python, HTML, MATLAB

Modeling Software: Amber 11, NAMD, Dock6, MOE, VMD, Chimera

Software development: co-developer of DOCK6.5 program.

E. Funding.

2008-pres. NIH National Research Service Award, Grant Number: 1F31CA134201-01, Characterizing the Mechanism of Cancer-Causing and Resistance Mutations of EGFR.