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Daniel P. Russo

Motivated, project-driven research scientist collaborating with academia, industry and government to develop non-animal alternatives for characterizing chemical toxicity or identifying drug candidates. Specifically, creating new computational approaches to exploit public and private data repositories to aid in the profiling of environmental and pharmaceutical compounds, including small molecules, peptides and nanoparticles. Background in designing and evaluating tools and methodologies to analyze chemical and biological data. Very passionate about scientific communication/teaching and inspired by scientists who discuss research in a clear, accessible manner.

Education

PhD 2014-2019 (Expected)
Computational & Integrative Biology, Rutgers University, Camden, NJ
Advised by Dr. Hao Zhu
Dissertation title: *Developing new approaches for screening chemical bioactivity using big data and deep learning*
Aug, 2019: Dissertation Awarded Distinction
Aug, 2019: Passed Comprehensive Exam with Distinction
March, 2016: Passed Qualifying Exam with Distinction
May, 2015: Completed Coursework, GPA: 3.96

MS 2011-2014
Biology, Rutgers University, Camden, NJ
Advised by Dr. Hao Zhu
Thesis: *Quantitative structure-activity relationship modeling of 5-hydroxytryptamine type-6 receptor antagonists*
March, 2014: Passed Thesis Defense with Distinction
May, 2013: Completed Coursework, GPA: 4.00

BA 2004-2009
Biology, Rutgers University, Camden, NJ

Experience

Employment

Rutgers University
Camden, NJ
Sept 2014-Present
Teaching/Graduate Assistant
Perform cheminformatics research in the lab of Dr. Hao Zhu. Develop statistical and machine learning models for toxicity and drug discovery. Lecture and grade students in courses related to Biology, Biochemistry, and Computer Science.

Collaborations Pharmaceuticals
Raleigh, NC
June 2017-Aug 2017
Intern
Developed predictive models for a variety of rare and neglected diseases and toxicity endpoints under the supervision of Dr. Sean Ekins. Trained and validated machine learning models using both classical algorithms and deep learning using Tensorflow/Keras on NVIDIA GeForce GTX 1080 GPUs.

West-Ward Pharmaceuticals
Cherry Hill, NJ
Sept 2013-Aug 2014
Microbiologist
Validated and performed experiments in the detection of microbial isolates and endotoxins from drug product and environmentally controlled manufacturing areas. Performed testing and recording in compliance with SOPs and cGMP regulations under FDA discretion.

Rutgers University
Camden, NJ
June 2012-Aug 2013
Part-time Lecturer/Certified College Reading & Learning Association Tutor
Lectured, graded, and tutored a variety of undergraduate level science courses in the fields of Biology, Biochemistry and Chemistry.

Adventure Aquarium
Camden, NJ
Sept 2008-Jan 2012
Biologist
Oversaw daily husbandry and animal health operations for a variety of marine, fresh, and brackish water fish and invertebrates. Assisted in diving and animal health operations for the 700,000-gallon Ocean Realm and 500,000-gallon Shark Realm exhibits featuring sharks, rays, turtles, and other large sea life. Educated visitors in marine science through guided tours and daily guest interactions.

Leadership Experience

Society of Toxicology - *In Vitro* and Alternative Methods Specialty Section
May 2019-Present

Vice Student Representative
Represent the students of the Society of Toxicology's *In Vitro* and Alternative Methods Specialty Section (IVAM-SS) by serving on the Executive Committee. Provide input at annual meetings to execute the mission, vision and values of IVAM-SS, which are rooted in developing non-animal models to toxicity testing.

Center for Computational & Integrative Biology Student Organizing Committee
May 2018-Present

Chair
Represent the interests of the Rutgers-Center for Computational & Integrative Biology (CCIB) Graduate Students through meetings with the CCIB Director and Graduate Program Director. Perform tasks as outlined in the CCIB Student Organizing Committee By-Laws including organizing student meetings, activities and other student-related social and academic events. Invite, host, and organize polling for student-elected seminar speakers.

Graduate Student Advisory Council
Sept 2016-Present

Council Member
Represent the interests of the Rutgers-Camden Graduate Students during meetings as part of an advisory group to the Associate Dean and Assistant Dean of the Graduate School. Assist with student orientation, open houses, and other graduate school programs.

Center for Computational & Integrative Biology Journal Club
Sept 2015-Present

Founder, Organizer
Select current and relevant papers in Computational Biology and assemble weekly meetings for discussion among CCIB students.

The Journal of Biological Sciences at Rutgers-Camden
Jan 2015-May 2015

Student Editor
Helped students prepare manuscripts for submission to faculty-reviewed scientific journal showcasing exceptional undergraduate research. Worked with both the students and the editor-in-chief to address reviewers' comments and finalize manuscripts for print.

Community Involvement

Software Carpentry
Sept 2016-Present

Instructor
Organize and host Software Carpentry workshops which aim to teach and describe a set of best practices for scientific software development that have solid foundations in research and experience.

The Academy of Natural Sciences Philadelphia, PA
Sept 2010-Sept 2013

Ichthyology Volunteer
Organized and curated the Ichthyology Collection consisting of close to 1.2 million catalogued specimens. Collected radiographic images (X-ray) of type specimens. Prepared and edited images using Adobe Photoshop.

Adventure Aquarium Camden, NJ
Aug 2005-Aug 2008

Fish & Invertebrates Volunteer
Assisted biology staff in daily husbandry and animal health operations for a variety of marine, fresh, and brackish fish and invertebrates.

Teaching Experience

All courses were taught at **Rutgers University**, Camden, NJ starting Sept 2012.
"Guest Lectures" are individual classes.

50:198:111 Programming Fundamentals Lab

50:198:113 Object-Oriented Programming Recitation

50:120:295 Principals and Practices of Biological Research

50:120:308 Genetics Lab

50:160:339 Organic Chemistry Lab

50:120:212 Microbiology and Its Applications Lab

50:120:107 General Biology Lab

56:115:511 Biochemistry I, *Guest Lecturer*: "Drug Discovery", "Sugars and Polysaccharides", "Protein Structures", "Aqueous Solutions", "Acids and Bases", "Nucleic Acids", "Proteins"

56:121:555 Cheminformatics, *Guest Lecturer*: "PubChem: Ushering Chemistry into 'Big Data'", "Public Chemical Databases"

Professional Membership

2018-Present American Society of Cellular and Computational Toxicology

2017-Present Society of Toxicology

2015-Present American Chemical Society

Certifications

2016 Software, Data, and Libraries Carpentry Instructor

2012 College Reading & Learning Association Tutor

2011 PADI Advanced Open Water Diver

2010 PADI Open Water Diver Certification

RESEARCH SKILLS

Computational

- Very good working knowledge of Python and object-oriented design specializing in scientific computing, specifically in the field of cheminformatics.
- Very good working knowledge of data science and data visualization using the Python packages Pandas, Numpy, SciPy, scikit-learn, Keras, matplotlib, and Bokeh.
- Proficient in machine learning principles and practices and their applications to chemistry, toxicology, and early stage drug discovery.
- Experience with a variety of computer tools and languages including bash, Git, Markdown, HTML, LaTeX, MongoDB, SQL, and web development using Flask.
- Very passionate about scientific communication and education. Host a blog titled "Drug Discovery in Python" showcasing data visualization and analysis within Python using chemistry and baseball as motivating fields.

Experimental

- Good experience with bacterial cell culture and aseptic technique with a strong focus on isolation and identification of bacteria and bacterial endotoxins.
- Experience with human cell culture (Hep G2) and assays.
- Good experience with a variety of biology and chemistry lab equipment and techniques including microscopy, high-pressure liquid chromatography, electrophoresis, DNA/RNA extraction, media buffer preparation, and various wet chemistry tests (pH, alkalinity, titrations).
- Good experience with fresh and marine fish and invertebrate care with a focus on the culture of various seahorse species: *H. erectus*, *H. reidi*, *H. abdominalis*, and *H. zosterae*.

PROJECTS & APPLICATIONS

CIIPro
Jan 2015-Present

Co-creator, developer, and maintainer of the *The Chemical In-vitro, In-vivo Profiling Project (CIIPro)*. CIIPro is an online cheminformatics web portal designed for large scale chemical and biological data analysis. CIIPro aims to harmonize the immense amount of data available in disparate public repositories for inclusion in cheminformatic studies. Written in Python and Flask, CIIPro is available at http://ciipro.rutgers.edu.

PubChemQSAR
Jan 2016-Present

Creator, developer, and maintainer of the open-source Python project *PubChemQSAR*. PubChemQSAR is a Python program that can build Quantitative Structure Activity Relationship (QSAR) models from any given biological assay from the chemical database PubChem. The program will extract assay data, prepare it for modeling, then use it to train a machine learning classifier from a variety of algorithms. The source code is available at http://www.github.com/russodanielp/PubChemQSAR.

FUNDING

Sept 2018 Center for Computational and Integrative Biology Travel Grant. $500.00

Sept 2018 Dean's Graduate Conference Travel Grant. $500.00

Mar 2018 Teaching Assistant and Graduate Assistant Professional Development Fund Award. $1,152.40

May 2017 2017-2018 Rutgers PhD Dissertation Fellowship. $5,000.00

Mar 2017 Teaching Assistant and Graduate Assistant Professional Development Fund Award. $1,000.00

Feb 2017 Center for Computational and Integrative Biology Travel Grant. $500.00

Feb 2017 Dean's Graduate Conference Travel Grant. $500.00

June 2016 Teaching Assistant and Graduate Assistant Professional Development Fund Award. $700.00

Jan 2010 Dean's Tuition Remission Award, Biology Department. $1,000.00

PUBLICATIONS & TALKS

Book Chapters

[1] **Russo D P** and Zhu H. Accessing the High-Throughput Screening Data Landscape. In: *High-Throughput Screening Assays in Toxicology* (by Zhu, H and Xia, M; Editors) Chapter 16, pgs. 153-159. Springer New York, 2015. ISBN: 978-1-4939-6344-7.

Articles

[1] **Russo D P**, Strickland J, Karmaus A L, Wang W, Shende S, Hartung T, Aleksunes L M, Zhu H. *Non-animal models for acute toxicity evaluations: applying data-driven profiling and read-across.* Environmental Health Perspectives. (2019) 127 (4), 047001. (**Selected as National Institutes of Environmental Health Science's Extramural Paper of the Month, June 2019.**)

[2] Ekins S, Puhl A C, Zorn K M, Lane T R, **Russo D P**, Klein J J, Hickey A J, Clark A M. *Exploiting machine learning for end-to-end drug discovery and development.* Nature Materials. (2019) 18, 435-441.

[3] Zorn K M, Lane T R, **Russo D P**, Clark A M, Makarov V, Ekins S. *Multiple machine learning comparisons of HIV cell-based and reverse transcriptase data sets.* Molecular Pharmaceutics. (2019) 16 (4), 1620-1632.

[4] Wang W, Yan X, Zhao L, **Russo D P**, Wang S, Liu Y, Sedykh A, Zhao X, Yan B, Zhu H. *Universal nanohydrophobicity predictions using virtual nanoparticle library.* J Cheminform. (2019) 18;11 (1), 6.

[5] **Russo D P**, Zorn K M, Clark A M, Zhu H, Ekins S. *Comparing multiple machine learning algorithms and metrics for estrogen receptor binding prediction.* Molecular Pharmaceutics. (2018) 15 (10), 4361-4370.

[6] Lane T R, **Russo D P**, Zorn K M, Clark A M, Korotcov A, Tkachenko V, Reynolds R, Perryman A L, Freunclich J S, Ekins S. *Comparing and validating machine learning models for Mycobacterium tuberculosis drug discovery.* Molecular Pharmaceutics. (2018) 15 (10), 4346-4360.

[7] Wang W, Sedykh A, Sun H, Zhao L, **Russo D P**, Zhou H, Yan B, Zhu H. *Predicting nano-bio interactions by integrating nanoparticle libraries and quantitative nanostructure activity relationship modeling.* ACS Nano. (2017) 11 (12), 12641-12649.

[8] Korotcov A, Tkachenko V, **Russo D P**, Ekins S. *Comparison of deep learning with multiple machine learning methods and metrics using diverse drug discovery data sets.* Molecular Pharmaceutics. (2017) 14 (12), 4462-4475.

[9] **Russo D P**, Kim M T, Wang W, Pinolini D, Shende S, Zhu H. *CIIPro: a new read-across portal to fill data gaps using public large-scale chemical and biological data.* Bioinformatics. (2016) 33 (3), 464–466.

[10] Xiang J, Zhang Z, Mu Y, Xu X, Guo S, Liu Y, **Russo D P**, Zhu H, Yan B, Bai X. *Discovery of novel tricyclic thiazepine derivatives as anti-drug-resistant cancer agents by combining diversity-oriented synthesis and converging screening approach.* ACS Combinatorial Science. (2016) 18 (5), 230-235.

[11] Yan B, Mu Y, Liu Y, Xiang J, Zhang Q, Zhai S, **Russo D P**, Zhu H, Bai X. *From fighting depression to conquering tumors: a novel tricyclic thiazepine compound as a tubulin polymerization inhibitor.* Cell Death and Disease. (2016) 7, e2143.

[12] Ball N, Cronin M T, Shen J, Adenuga M D, Blackburn K, Booth E D, Bouhifd M, Donley E, Egnash L, Freeman J J, Hastings C, Juberg D R, Kleensang A, Kleinstreuer N, Kroese E D, Luechtefeld T, Maertens A, Marty S, Naciff J M, Palmer J, Pamies D, Penman M, Richarz A N, **Russo D P**, Stuard S B, Patlewicz G, van Ravenzwaay B, Wu S, Zhu H, Hartung T. *Toward Good Read-Across Practice (GRAP) guidance.* ALTEX. (2015) 33, 149-166. **(Featured together with the following 4 ALTEX papers in Science Feb 12, 2016 "A crystal ball for chemical safety" and Nature Feb 11, 2016 "Legal tussle delays launch of huge toxicity database")**

[13] Luechtefeld T, Maertens A, **Russo D P**, Rovida C, Zhu H, Hartung T. *Analysis of publicly available skin sensitization data from REACH registrations 2008-2014.* ALTEX. (2015) 33, 135-148.

[14] Luechtefeld T, Maertens A, **Russo D P**, Rovida C, Zhu H, Hartung T. *Analysis of Draize eye irritation testing and its prediction by mining publicly available 2008-2014 REACH data.* ALTEX. (2015) 33, 123-134.

[15] Luechtefeld T, Maertens A, **Russo D P**, Rovida C, Zhu H, Hartung T. *Analysis of public oral toxicity data from REACH registrations 2008-2014.* ALTEX. (2015) 33, 111-122.

[16] Luechtefeld T, Maertens A, **Russo D P**, Rovida C, Zhu H, Hartung T. *Global analysis of publicly available safety data for 9,801 substances registered under REACH from 2008-2014.* ALTEX. (2015) 33, 95-109.

[17] Kotchoni, S O, Noumavo, P A, Adjanohoun A, **Russo D P**, Dell Angelo J, Gachomo E W, Baba-Moussa L. *A simple and efficient seed-based approach to induce callus production from B73 maize genotype.* American Journal of Molecular Biology. (2012) 2, 380-385.

Presentations

Mar 2019 *Extensive data-driven modeling of food-derived bioactive peptides that inhibit the angiotensin I-converting enzyme.* American Chemical Society Annual Meeting - Division of Chemical Information, Orlando, FL

Sept 2018 *Developing mechanism-based animal toxicity models: A chemocentric approach using big data.* 7th Annual Meeting of the American Society for Cellular and Computational Toxicology,· Bethesda, MD†

Apr 2018 *Multitask deep neural networks for prediction of estrogen receptor activity.* Center for Computational and Integrative Biology Spring Seminar, Camden, NJ

Dec 2017 *Developing mechanism-based toxicity models from big data.* Center for Computational and Integrative Biology Annual Retreat, Camden, NJ

Sept 2016 *CIIProCluster: Developing enhanced predictive toxicity models using big data.* Center for Computational and Integrative Biology Fall Seminar, Camden, NJ

Sept 2015 *CIIPro: An online cheminformatics portal for large scale chemical data analysis.* Center for Computational and Integrative Biology Fall Seminar, Camden, NJ

Aug 2015 *CIIPro: An online cheminformatics portal for large scale chemical data analysis.* American Chemical Society Annual Meeting - Division of Chemical Information, Boston, MA

May 2013 *Quantitative structure activity relationship modeling of serotonin type-6 receptor antagonists.* Rutgers-Camden Biology Spring Seminar, Camden, NJ

†Winner of the Tox21 Student Award for best presentation and profiled on the Rutgers website: "Computational and Integrative Biology Doctoral Student Daniel Russo Receives Tox21 Student Award"

Posters

** *poster presenter*

Dec 2018 **Russo D P, Zhang Y, Zhu H. *Extensive data-driven modeling of food-derived bioactive peptides that inhibit the angiotensin I-converting enzyme.* Center for Computational and Integrative Biology Annual Retreat - Rutgers University, Camden, NJ

Apr 2018 **Russo D P, Ciallella H L, Zorn K, Ekins S, Zhu H. *Multi-class deep neural network modeling of US EPA categorized rat acute oral toxicity.* Predictive Models for Acute Oral Systemic Toxicity Workshop - National Institutes of Health, Bethesda, MD

Apr 2018 Ciallella H L, **Russo D P**, Zorn K, Clark A M, Korotcov A, Tkachenko V, Ekins S, Zhu H. *Consensus quantitative structure-activity relationship modeling for rat acute oral toxicity endpoints.* Predictive Models for Acute Oral Systemic Toxicity Workshop - National Institutes of Health, Bethesda, MD

Mar 2018 **Russo D P, Zorn K, Clark A M, Korotcov A, Tkachenko V, Zhu H, Ekins S. *Comparison of multiple machine learning algorithms, descriptors and metrics for estrogen receptor binding.* Society of Toxicology Annual Meeting, San Antonio, TX

Apr 2017 **Russo D P, Wang W, Strickland J, Shende S, Hartung T, Zhu H. *CIIProCluster: Developing read-across predictive toxicity models using big data.* Celebration of Graduate Research - Rutgers University, Camden, NJ

Mar 2017 **Russo D P, Wang W, Strickland J, Shende S, Hartung T, Zhu H. *CIIProCluster: Developing read-across predictive toxicity models using big data.* Society of Toxicology Annual Meeting, Baltimore, MD

Mar 2017 Wang W, Sedykh A, Sun H, Zhao L, **Russo D P**, Yan B, Zhu H. *Virtual gold nanoparticle library: simulation, modeling, and experimental validation.* Society of Toxicology Annual Meeting, Baltimore, MD

Dec 2016 **Russo D P, Wang W, Strickland J, Shende S, Zhu H. *CIIProCluster: Developing read-across predictive toxicity models using big data.* Center for Computational and Integrative Biology Annual Retreat - Rutgers University, Camden, NJ

Mar 2016 Wang W, **Russo D P**, Kim M T, Zhao L, Huang R, Xia M, Hartung T, Zhu H. *Profiling and evaluating environmental chemicals that induce oral acute toxicity using mitochondrial membrane potential disruption assay, Big Data and New Read-across Strategy.* Society of Toxicology 55th Annual Meeting, New Orleans, LA

Sep 2015 **Russo D P, Wang W, Kim M T, Pinolini D, Zhu H. *CIIPro: An online cheminformatics portal for large scale chemical data analysis.* Center for Computational and Integrative Biology Annual Retreat - Rutgers University, Camden, NJ

Aug 2015 **Russo D P, Wang W, Kim M T, Pinolini D, Zhu H. *CIIPro: An online cheminformatics portal for large scale chemical data analysis.* Sci-Mix Poster Session, American Chemical Society - Division of Chemical Information, Boston, MA

Sept 2013 Kim T M, Lallier B, Zhang J, **Russo D P**, Mayer-Bacon C, Boison A, Kotchoni S O, Martin J V, Zhu H. *Computational profiling of the binding mechanisms of GABAA receptor ligands.* American Chemical Society Annual Meeting- Division of Chemical Information, Indianapolis, IN

Workshops & Panels

Feb 2019 *Panelist*, Award Winners Series: Combining Biological and Computational Approaches - American Society for Cellular and Computational Toxciology Webinar

Feb 2019 *Organizer & Lead Instructor*, Software Carpentry Workshop - Rutgers University, Camden NJ

Oct 2017 *Organizer & Lead Instructor*, Software Carpentry Workshop - Rutgers University, Camden NJ

Nov 2016 *Organizer & Instructor*, Software Carpentry Workshop - Rutgers University, Camden NJ

Mar 2016 *Panelist*, Admitted Students Day Panel - Rutgers University, Camden NJ

Oct 2016 *Panelist*, Good Read-Across Practices Workshop - Johns Hopkins Center for Alternatives to Animal Testing, Baltimore, MD

Media & Press

An end to animal testing?, Science Node. June 16, 2019.

New algorithm could save thousands of animals from toxic testing., Silicon Republic. April 17, 2019.

Can an algorithm replace animal testing for chemicals?, Futurity. April 17, 2019.

New algorithm allows for faster, animal-free chemical toxicity testing, Science Daily. April 16, 2019.

Rutgers team predicts toxicity by mining PubChem data, Chemical Watch. April 16, 2019.

Young Scientist Spotlight, Interview by Nikaeta Sadekar. American Society of Cellular and Computational Toxicology Newsletter. Volume IX, Issue I.