Jacob O. Spiegel, Ph.D.

jspiegel@pitt.edu (516) 984-7751 linkedin.com/in/Jacob-Spiegel-PhD/ Jacob-Spiegel.github.io/

10+ years of computational and wet lab scientific research experience. Expertise includes cheminformatics, computational drug discovery, Python tool development, pharmaceutical informatics, and data visualization. Looking for opportunities to develop enterprise solutions and lead teams that optimize drug design workflows.

Professional Experience

Exscientia AI, *Cheminformatic Research Engineer* 2021 – present
Miami, Florida
- Developing and maintaining cheminformatic toolkits, software, and workflows
- Serving as Cheminformatic lead on drug design team
- Serving as Cheminformatic software developer on generative design product team

Workflow Informatics Corp., *Research Informatics Consultant/V.P. of Product Development* 2020 – 2021
- Developed informatics, visualizations, and research solutions for pharmaceutical companies
- Independently managed 15 clients ranging from startup to enterprise-sized organizations with an active client load of 5-8 clients per month
- Developed an algorithm for heterocyclic regioisomer enumeration
- Managed version-controlled QSAR model repository and cross-platform model integration
- Automated data workflows and removed manual curation for data-synchronization
- Oversaw data migrations (e.g., ELN, compound registry, and assay data)
- Trained and managed a team of two junior consultants

Education

University of Pittsburgh 2014 – 2020
Ph.D in Molecular Biophysics and Structural Biology Pittsburgh, PA
- Thesis title: "Targeting the Poly (ADP-Ribose) Polymerase-1 Catalytic Pocket Using AutoGrow4, a Genetic Algorithm for *De Novo* Design"

Ph.D Minor in Teaching

Carnegie Mellon University 2013 – 2014
Ph.D. Student in Molecular Biophysics and Structural Biology Pittsburgh, PA

Stony Brook University 2009 – 2013
B.Eng. in Biomedical Engineering - Cellular and Molecular Biology Track Stony Brook, NY

Research Experience

University of Pittsburgh 2013 – 2020
Ph.D. Candidate/Researcher in Dr. Jacob Durrant's laboratory Pittsburgh, PA
- Designed, developed, documented, and maintained five Python open-source programs for computer-aided drug design (CADD) and cheminformatics; parallelized code for multiprocessing
- Applied CADD techniques to biological targets; performed molecular dynamic (MD) and weighted ensemble MD simulations on multiple proteins; performed protein homology modeling
- Mentored, managed, and designed projects with undergraduate labmates

Ph.D. Candidate in Dr. Roger Hendrix's laboratory
- Studied bacteriophages using biochemical, molecular genetic, and X-ray crystallography techniques
- Collaborated on cryo-EM reconstruction of bacteriophage λ tail proteins
- Engineered plasmids; designed protein purification protocols; X-ray crystallography

Stony Brook University 2011 – 2013
Undergraduate Researcher in Dr. Balaji Sitharaman's laboratory Stony Brook, NY
- Studied nanoparticle drug delivery system targeting cancer cells
- Designed alternative exfoliation protocol to produce graphene sheets from graphite

Cold Spring Harbor Laboratory 2007 – 2010
Researcher in Dr. Jonathan Sebat's laboratory Woodbury, NY
- Semi-Finalist, Intel Science Talent Search
- Designed and conducted independent population genetic study
- Performed microarray studies searching for polymorphism in autism and bipolar disorder

Pro Bono Research

Research Advisor 2020 – Current
- Advised student at University of Havana in developing and implementing a study to determine the most effective molecular docking programs for various protein pockets, including the Malaria metalloprotein PfA-M1 aminopeptidase Havana, Cuba
- Established an international collaboration between the University of Havana and the University of Pittsburgh
- Contributed to Python codebase, experimental design, and paper writing

DataKind, *Volunteer Data Engineer* 2020 – 2021
- Aided in data munging and visualization for Red Cross Fire Risk Mapping

Leadership and Outreach

Sigma Phi Delta Engineering Fraternity 2010 – Current
- International Scholastic Development Manager
- Founding member of the Beta-Eta Chapter at Stony Brook University
- Rush Chairman, Sergeant at Arms, Alumni Relations Manager, Risk Reduction Manager, Initiate Education and Academic Chairman

Mars Elementary School Science Fair 2018 – 2019
- Volunteer judge at Mars Elementary School Science Fair 2018 & 2019 Mars, PA

Engineers Without Borders USA 2010 – 2013
- Founding Member of the Stony Brook University chapter
- Project Development Manager

Awards

Abe and Jean Comensky Memorial Scholarship 2019

Amdursky Scholarship 2019

Biomedical Graduate Student Association Travel Award University of Pittsburgh 2018
- Awarded for oral presentation at RDKit UGM 2018 at Cambridge University, Cambridge, England

Publications

Peer-Reviewed Articles
- **Spiegel, J.O.**, et al. PARP1: Structural insights and pharmacological targets for inhibition. DNA Repair 103 (2021). https://doi.org/f9x2
- **Spiegel, J.O.**, Durrant, J.D. AutoGrow4: an open-source genetic algorithm for *de novo* drug design and lead optimization. J Cheminform 12, 25 (2020). http://doi.org/ggwwcp
- Ropp, P.J., **Spiegel, J.O.**, et al. Gypsum-DL: an open-source program for preparing small-molecule libraries for structure-based virtual screening. J Cheminform 11, 34 (2019). http://doi.org/gf48dh

Articles in Preparation
- **Spiegel, J.O.**, O'Donnell, A., Durrant, J.D., (2023). Molecular dynamics of α-arrestin TXNIP.
- **Spiegel, J.O.**, Durrant, J.D., Bowman, R., O'Donnell, A. (2023). Putting the brakes on α-arrestin trafficking: α-arrestin regulation by phosphorylation and ubiquitination.
- Mayo, E., **Spiegel, J.O.**, Durrant, J.D., Ochoa, E (2023). Evaluation of metalloprotein docking using Plasmodium falciparum PfA-M1 aminopeptidase.
- **Spiegel, J.O.**, Lowden, C., (2023). A novel approach for heterocyclic regioisomer enumeration.

Acknowledgement of Contribution

- Kappler, M., Lowden, C. and Culberson, J. (2022) BioChemUDM: a unified data model for compounds and assays. Pure and Applied Chemistry, Vol. 94 (Issue 6), pp. 737-744. https://doi.org/10.1515/pac-2021-1004
- Durrant, J. D. (2019). Blendmol: Advanced macromolecular visualization in Blender. Bioinformatics, 35(13), 2323–2325. https://doi.org/10.1093/bioinformatics/bty968

Patents

- **Spiegel, J.O.**, Lalwani, G., Toussaint, J., Patel, S., Sitharaman, B. (2013). Synthesis of Graphene Via Hydro-Jets. US Provisional Application, OTLIR, Stony Brook University

Conference Presentations

Oral Presentations

- **Spiegel, J.O.** "Automated Analog Generation and Retrosynthesis Predictions" Oral presentation at the 10th RDKit UGM 2021, October 14th, 2021
- **Spiegel, J.O.**, Ropp, P.J., and Durrant, J.D. "Autogrow 4.0: Improved Genetic Algorithm for *de novo* Computer Aided Drug Design" Oral presentation at the MBSB 2018 Symposium, University of Pittsburgh, Pittsburgh PA May 18, 2018

Poster Presentations

- **Spiegel, J.O.**, Ropp, P.J., and Durrant, J.D. "Autogrow 4.0: Improved Genetic Algorithm for *de novo* Computer Aided Drug Design" Poster presentation at the MBSB 2019 Symposium, University of Pittsburgh, Pittsburgh PA May 13, 2019
- **Spiegel, J.O.**, Duda, R., and Hendrix, R. "Structure determination of λ Tail Assembly Chaperone" Poster presentation at the XXV 2017 Conference on Phage and Virus Assembly, Ellicott City, Maryland August 23, 2017
- **Spiegel, J.O.**, Duda, R., and Hendrix, R. "Structure determination of λ Tail Assembly Chaperone" Poster presentation at the MBSB 2017 Symposium, University of Pittsburgh, Pittsburgh PA May 19, 2017
- **Spiegel, J.O.**, Duda, R., and Hendrix, R. "Structure of λ Tail Assembly Chaperone" Poster presentation at the MBSB 2016 Symposium, University of Pittsburgh, Pittsburgh PA May 13, 2016
- **Spiegel, J.O.**, Duda, R., and Hendrix, R. "ΦHau3 Ribosomal Bypass Mechanism" Poster presentation at the MBSB 2015 Symposium, University of Pittsburgh, Pittsburgh PA May 15, 2015

Teaching Experience

Pro Bono Mentoring 2020 – 2021
Research Advisor Havana, Cuba

- Worked with students from the University of Havana to develop a research project and an Individualized Development Plan (IDP)
- Weekly code and writing reviews; Python and structural biology training

University of Pittsburgh 2018 – 2020

Ph.D. Minor in Teaching (2018-2020) Pittsburgh, PA

- A two-year graduate-level program. The program included pedagogy training, teaching mentoring, and teaching experience

Guest Lecturer: Computational Biology Research (January 31, 2020)

- A three-hour-long lecture of 25 students. Designed lesson plan and homework assignment, administered lesson and coordinated in-class discussion using active learning techniques, and designed exam questions for the final
- Coarse covered an intermediate level of Python coding, with focuses in using third-party APIs including RDKit, Numpy, and Scipy. This lesson also detailed Python Enhancement Proposals (PEP) practices and introduced the core concepts of cheminformatics

Undergraduate Research Mentor (Fall 2018 – Fall 2019)

- Held weekly supervision meetings, assisted in project design and code reviews culminating in mentee's authorship on the Gypsum-DL paper (2019)

Guest Lecturer: Computational Biology (March 21, 2019)

- Hour-long lecture of 25 students. Designed lesson plans and homework assignments, administered lessons and coordinated in-class discussion using active learning techniques, and designed exam questions for the final
- Course covered protein druggability, tools for predicting project success rate, rare and tropical diseases, drug toxicity, drug specificity

Graduate Teaching Assistant: Biochemistry Lab (Spring 2019)

- Two separate lab sessions of a combined 38 students. Designed lectures and experiments for the class, designed assignments, graded notebooks and assignments, and prepared materials for in-class experiments
- Course covered aseptic technique, cloning, fusion protein construct, protein induction in E. coli, protein purification, gel electrophoresis, lab notebooks

Graduate Teaching Assistant: Macromolecular Structure and Function (Fall 2018)

- Weekly lectures and four separate recitation sections for 100 students. Designed lectures and lesson plans, managed undergraduate teaching assistants, and graded papers
- Course covered fundamentals of structural biology, enzyme catalysis, proteomics, fundamentals of biochemistry

Guest Lecture: Biochemistry Lab (February 26, 2018)

- Two hour-long lectures with a total of 38 students. Designed lesson plans and homework assignments, administered lessons
- Lesson was to overview virology, focusing on the classification of virus, viral structure and function, and describe the phage HK97, which students would be studying throughout the semester.

Graduate Teaching Assistant: Biochemistry Lab (Spring 2018)

- Two lab sessions with a total of 38 students. Designed lectures and experiments for the class, designed assignments, graded notebooks and assignments, and prepared materials for in-class experiments
- Course covered phage biology, aseptic technique, cloning, fusion protein construct, protein induction in E. coli, protein purification, gel electrophoresis, lab notebooks

Carnegie Mellon University 2014 – 2014

Graduate Teaching Assistant: Virology (Spring 2014) Pittsburgh, PA

- Class of 50 students. Conducted recitations, aided in lectures, and graded assignments and exams.
- Course covered bacteriophage biology, mammalian virology, lytic/lysogenic states, virus-caused diseases

Computation Skills and Experience

Python
Expert in Python Programming, RDKit, and OpenEye

Pipeline Pilot - BIOVIA
Developed Custom Commercial Programs

StarDrop - Optibrium
Developed Custom Integrated Applications and Visualizations

TIBCO Spotfire
Developed Custom Integrated Applications and Visualizations

ELN Management
Supervised Selection, Deployment, and ELN Migrations

Compound/Data Registration and Management
CDD Vault, Visualize scigilian, Oracle, and SQL

Molecular Docking
5+ Years Experience Customizing Docking Workflows

Molecular Dynamics Simulations
NAMD and Weighted Ensemble Simulation (WESTPA)

Certifications

Machine Learning by Andrew Ng
06/2022 – 09/2022
Stanford University