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
- 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; purified proteins for 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

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

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.

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

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)