

Sebastian Raschka

Contact Information

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Education

- 2012-present** Ph.D. candidate Biochemistry & Molecular Biology and Quantitative Biology
Dual-major Ph.D. - Michigan State University
- Main research topics:
1) *High-throughput virtual screening for antagonist and agonist discovery.*
2) *Near-native binding mode prediction by rigidity analysis of protein-ligand complexes.*
3) *Discovery and characterization of patterns of preferential interactions between proteins and their ligands.*
- Advisor: Prof. Dr. Leslie A. Kuhn
- 2008-2012** B.Sc. Biology Plus International - Heinrich-Heine-Universitaet Duesseldorf
- Thesis: *Investigation of potential CLAVATA2 interactors by Fluorescence Resonance Energy Transfer Analysis*
- Advisor: Prof. Dr. Ruediger Simon
- 2011-2012** Study Abroad - Michigan State University
- Research during the 1st semester: *Acetylation-dependent SUMOylation of p53*
Advisor: Prof. Dr. Min-Hao Kuo
- Research during the 2nd semester: *Phylogenetic studies of Rhagoletis flies and associated parasitoid Coptera wasps*
Advisor: Prof. Dr. Jim Smith
- 1996-2007** High School Diploma - Gymnasium Rheinkamp Europaschule Moers

Professional Experience and Employment History

2012-present Protein Structural Analysis & Design Lab Prof. Kuhn
Graduate Research Assistant

Collaborated with experimental biologists (MSU Department of Fisheries and Wildlife) and designed machine learning models in time-sensitive projects to successfully predict receptor antagonists of sea lamprey mating pheromones. We discovered inhibitors that could block 93% of pheromone reception at 10^{-9} M concentration in electro-olfactogram assays and at 10^{-12} M concentration in natural water streams.

Developed a hypothesis-driven methodology and Python software framework, Screenlamp, for large-scale virtual screening allowing researchers to identify target molecules of protein receptors at an unprecedented scale in databases of more than 15 million compounds.

Developed algorithms and a Python/C software package, SiteInterlock, for predicting 3-dimensional protein-ligand binding poses on the time scale of seconds with a predictive accuracy equal to existing approaches. This novel approach is based on the hypothesis that interfacial rigidification of both the protein and ligand prove to be important characteristics of the native binding mode and are sensitive to the spatial coupling of interactions and bond-rotational degrees of freedom in the interface.

Managed IT systems in the Kuhn lab, including hardware, software, servers, computing clusters, and Linux workstations.

2017-present Joint Research Collaboration with the MSU i-PRoBe Lab
Research Collaborator

Designed and implemented a novel artificial neural network architecture for deep learning based on ideas from the field of general adversarial networks with applications to facial recognition and biometrics.

May 2012-Aug 2012 Computational Pharmaceutical Chemistry Lab Dr. Holger Gohlke
Research Internship

Research project: *Analysis of protein thermostability using a constraint network approach based on graph theory.*

Conducted molecular dynamics simulations and analyzed the resulting trajectories to predict the effect of binding-site mutations on the thermostability of various proteins.

May 2010-Oct 2010 Immulab Duesseldorf
Internship

Performed computational and statistical analyses of real-time qPCR data from human saliva samples to diagnose paradontose causing bacteria.

**Oct 2007-
Mar 2008** St. Thekla home for the elderly, Rheinberg, Germany
Community Service

Assisted the elderly with household tasks and the participation in social activities.

Teaching Experience

Aug 2016 Machine Learning with scikit-learn at SciPy 2016, Austin, Texas
Instructor

Taught an 8-hour workshop on machine learning and scikit-learn (approx. 50 participants).

**May 2014-
Jul 2014** BMB 401: Comprehensive Biochemistry, Michigan State University
Graduate Teaching Assistant

Held weekly office hours and organized weekly study groups to help students with the course material. Co-supervised examinations (approx. 300 students).

**Jun 2010-
Aug 2010** Bio 250: Genetics, Heinrich-Heine Universitaet Duesseldorf
Student Teaching Assistant

Co-supervised laboratory sessions and designed evaluated weekly written tests to help students with the course material and preparation for the exam (approx. 200 students).

Honors and Awards

- *MSU BMB Outstanding Graduate Student Award (2016-2017)*

Clubs/Extracurricular Activities

**Oct 2016-
present** MSU Data Science Club
Member and speaker

Advised MSU students in applying data science techniques to research problems.

- Jan 2017-
June 2017** Udacity Deep Learning Nanodegree
Continued education
- Completed a 16-week course implementing various deep neural networks for text and image recognition and generation.
- Oct 2013-
Apr 2014** Council of Graduate Students, Michigan State University
Departmental Representative
- Participated in council meetings and discussions, representing the Department of Biochemistry and Molecular Biology.

Technical Skills

- *Computational biology and structural modeling*
Expert in using protein-ligand docking tools and protein-ligand scoring functions for pose-prediction and conducting large-scale ligand-based virtual screenings for agonist/antagonist discovery. Other skills include the use of molecular dynamics simulations, energy minimization, protonation and charge assignment, conformer analysis, 3-dimensional structure alignments and pharmacophore detection, homology modeling, and multiple sequence alignments (amino acid sequences and DNA) in research projects. Trained and helped supervise undergraduate research assistants and graduate rotation students.
- *Machine learning and deep learning*
Author of the best-selling book *Python Machine Learning, Packt Publishing Ltd., 2015* and instructor of various machine learning workshops. Expert knowledge in parametric and non-parametric modeling for supervised learning. Expert knowledge in unsupervised learning, including clustering, dimensionality reduction, and manifold learning. Good familiarity with TensorFlow and capable of implementing deep artificial neural networks, including convolutional neural networks and recurrent neural networks with long short term memory, from scratch for large-scale image classification and speech recognition on distributed systems.
- *Statistics and probability theory*
Experienced in using various statistical analyses, including frequentist methods for hypothesis testing and pattern recognition based on Bayesian decision theory.
- *Large-scale data analysis and visualization*
Analysis of small and large datasets, primarily using Python libraries (matplotlib and seaborn) and R.
- *High performance computing*
User of the High Performance Computing Cluster (HPCC) at Michigan State University and Amazon EC2 for high-throughput virtual screening and machine learning applications.
- *Git version control*
Multi-year experience in reproducible research and the development and maintenance of open source projects under version control via GitHub and GitLab.

- *Programming Languages*
Python (very strong knowledge, preferred language for scientific programming)
R, C, Bash, SQL, HDF5 (strong knowledge)
C++, JavaScript, HTML, CSS (good knowledge)
Java, Scala (basic knowledge)

First Author Publications

Books

- Raschka, Sebastian *Introduction to Artificial Neural Networks and Deep Learning (In prep.)* [<https://github.com/rasbt/deep-learning-book>].
- Raschka, Sebastian, Vahid Mirjalili. *Python Machine Learning. 2nd Edition.* Birmingham, UK: Packt Publishing, 2017. (*In prep.*)
- Raschka, Sebastian, David Julian, and John Hearty. *Python: Deeper Insights into Machine Learning.* Birmingham, UK: Packt Publishing, 2016. ASIN: B01LD8K994.
- Raschka, Sebastian. *Python Machine Learning.* Birmingham, UK: Packt Publishing, 2015. ISBN: 978-1783555130. (Amazon bestseller in Data Mining 2015 & 2016, Packt bestselling title 2015 & 2016, more than 45,000 copies sold)
- Raschka, Sebastian. *Python Machine Learning (Korean Transl.)*. Korea: Ji & Son, 2017. ISBN: 979-1187497035.
- Raschka, Sebastian. *Machine Learning mit Python (German Transl.)*. Frechen, Germany: mitp Verlag, 2016. ISBN: 978-3958454224.
- Raschka, Sebastian. *Machine learning con Python. Costruire algoritmi per generare conoscenza (Italian Transl.)*. Italy: Guida Completa, 2016. ISBN: 978-8850333974.
- Raschka, Sebastian. *Python Machine Learning (Japanese Transl.)*. Japan: Impress Top Gear, 2016. Japanese: 978-4844380603.
- Raschka, Sebastian. *Python Machine Learning (Chinese Transl.)*. New Taipei City, Taiwan: DrMaster Press Co., Ltd., 2016. ISBN: 978-9864341405.
- Raschka, Sebastian. *Heat Maps in R: How-To.* Birmingham, UK: Packt Publishing, 2013. ISBN: 978-1782165644. (more than 500 copies sold)

Book Chapters

- Raschka, Sebastian, Leslie A. Kuhn, Anne M. Scott, and Weiming Li. *Computational Drug Discovery and Design: Automated Inference of Chemical Group Discriminants of Biological Activity from Virtual Screening Data.* Springer, 2017. (*In prep.*)

Peer Reviewed Journals

- Raschka, Sebastian, Alex Wolf, and Leslie A. Kuhn. *Patterns of preferential interactions between proteins and their ligands*. [manuscript in preparation]
- Raschka, Sebastian, Nan Liu, Santosh Gunturu, Anne M. Scott, Mar Huertas, Weiming Li, and Leslie A. Kuhn. *Facilitating the hypothesis-driven prioritization of small molecules in large databases: Screenlamp and its application to GPCR inhibitor discovery*. [submitted]
- Raschka, Sebastian. *BioPandas: Working with molecular structures in pandas DataFrames*. The Journal of Open Source Software 2.14 (2017).
- Raschka, Sebastian, Joseph Bemister-Buffington, and Leslie A. Kuhn. *Detecting the native ligand orientation by interfacial rigidity: SiteInterlock*. Proteins: Structure, Function, and Bioinformatics 84.12 (2016): 1888-1901.

Preprints

- Raschka, Sebastian. *MusicMood: Predicting the mood of music from song lyrics using machine learning*. arXiv preprint arXiv:1611.00138 (2016).
- Raschka, Sebastian. *Naive Bayes and Text Classification I-Introduction and Theory*. arXiv preprint arXiv:1410.5329 (2014).

Selected Oral Presentations

- Raschka, Sebastian, J. Bemister-Buffington, and L.A. Kuhn. *Binding pose prediction via rigidity analysis and large-scale pheromone antagonist discovery for invasive species control*. MSU Computational and Systems Biology Journal Club. Mar 2017. East Lansing, MI.
- Raschka, Sebastian. *Machine Learning and Performance Evaluation – Overcoming the Selection Bias*. DataPhilly. Nov 2016. Philadelphia, PA.
- Raschka, Sebastian, J. Bemister-Buffington, and L.A. Kuhn. *Detecting the Native Ligand Orientation by Interfacial Rigidity*. BMB Departmental Retreat. Oct 2016. Okemos, MI.
- Raschka, Sebastian. *Getting Started with Data Science*. MSU DataScience. Sep 2016. East Lansing, MI.
- Raschka, Sebastian. *Learning Scikit-Learn*. PyData 2016. Aug 2016. Chicago, IL.
- Raschka, Sebastian, and A. C. Mueller. *Machine Learning with Scikit-Learn*. SciPy 2016. Jul 2016. Austin, TX.
- Raschka, Sebastian, J. Bemister-Buffington, and L.A. Kuhn. *A Novel Approach to Protein-Ligand Binding Mode Prediction by Rigidity Analysis Using Graph Theory*. Biomolecular Science Gateway. Feb 2016. East Lansing, MI.

- Raschka, Sebastian. *Practical Data Science. An Introduction to Supervised Machine Learning and Pattern Classification*. MSU NextGen Bioinformatics. Feb 2015. East Lansing, MI.
- L. A. Kuhn, N. Liu, A. Scott, S. Gunturu, S. Raschka, M. Huertas, and W. Li, *Screening and Identifying Pheromone Receptor Antagonists for Invasive Species Control*, ACS Division of Environmental Chemistry Session: Great Lakes Restoration Initiative: An Environmental Chemistry Challenge”, 248th ACS National Meeting and Exposition San Francisco, CA, August 10-14, 2014

Poster Presentations

- S. Raschka, N. Liu, S. Gunturu, A.M. Scott, M. Huertas, W. Li, and L.A. Kuhn *Screenlamp: A Software Framework for Hypothesis-Driven Ligand Discovery Based on Virtual Screening and Machine Learning*. Great Lakes Bioinformatics and Canadian Computational Biology Conference 2016, University of Toronto, May 16-19, 2016
- A. Scott, M. Huertas, S. Raschka, N. Liu, L.A. Kuhn, and W. Li, *Regulation of Pheromone Induced Responses with Behavioral Antagonists for Invasive Sea Lamprey (*Petromyzon marinus* L.) Control*. Behaviour 2015 conference, Cairns, Australia, August 8, 2015
- S. Raschka, N. Liu, S. Gunturu, A.M. Scott, M. Huertas, W. Li, and L.A. Kuhn, *A Hypothesis-Driven Virtual Screening Methodology for Structure-Based Inhibitor Discovery*. Quantitative Biology Symposium, Michigan State University, East Lansing, August 18, 2014
- A. Scott, M. Huertas, N. Liu, S. Gunturu, S. Raschka, L. A. Kuhn, and W. Li, *Identification of pheromone receptor antagonists for invasive sea lamprey control*. International Congress on the Biology of Fish, Heriot-Watt University, UK, 3-7 August, 2014

Peer Reviewing

- American Chemical Society (ACS) Publications
- The Journal of Open Source Software (JOSS)

Open Source Projects

- Contributor to the Python machine learning library scikit-learn
- Contributor to the deep learning library TensorFlow
- Creator and maintainer of the Python data science library mlxtend

- Creator and maintainer of BioPandas, a Python package for working with molecular structures via data frames
- Member of the conda-forge organization, which provides recipes, build infrastructure, and distributions for the conda package manager
- An extended open source portfolio is available on GitHub: <https://github.com/rasbt>

Selected Journalism Contributions

- KDnuggets, 2016: *Top 2016 KDnuggets Stories*
- KDnuggets, 2016: *Data Preparation Tips, Tricks, and Tools: An Interview with the Insiders*
- Huffington Post, 2016: *The Impact of Machine Learning on Healthcare*
- Forbes, 2016: *What Do Computational Biologists Do?*
- Hacker Bits print magazine, 2016: *Everyone is talking about deep learning these days, but what the heck is it?*
- Open Data Science, 2016: *Trifecta: Python, Machine Learning, and Dueling Languages A.I.*
- Open Data Science, 2016: *Model Evaluation, Model Selection, and Algorithm Selection in Machine Learning*
- Partially Derivative Podcast Interview, 2017: *Model Evaluation with Sebastian Raschka*
- Data Science at Home Podcast Interview, 2016: *30 min with data scientist Sebastian Raschka*
- Becoming a Data Scientist Podcast, 2016: *30 min with data scientist Sebastian Raschka*

Selected Press Coverage

- A.I. & Optimization, 2016: *Top 22 Python Programming Books*
- KDnuggets, 2016: *Top 10 Essential Books for the Data Enthusiast*
- KDnuggets, 2016: *5 Machine Learning Projects You Can No Longer Overlook*
- Techopedia, 2016: *Artificial Intelligence: Experts To Follow on Twitter*
- InformationWeek, 2016: *10 Big Data Books To Boost Your Career*
- OpenSource.org, 2015: *Publisher's picks: 29 open source books for 2015*
- Datawerq, 2015: *50 Data leaders to follow on Twitter*

- Onanalytica, 2015: *Artificial Intelligence & Machine Learning: Top 100 Influencers and Brands*
- Analytics Vidhya, 2015: *Top Data Scientists to follow on GitHub*