Jenke Scheen

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github | linkedin

Summary

Goal-oriented computational chemistry scientist with 7+ years of experience in applying modern solutions to academic drug discovery projects. Biologist by training and enjoys applying algorithmic solutions to hit optimisation problems in early drug discovery as well as developing existing methodologies to further push the boundaries of computational chemistry. Seeking to diverge into a professional setting to apply knowledge gained in academia to real-world drug discovery efforts.

Experience

Memorial Sloan Kettering Cancer Center

2022- / New York, USA

Postdoctoral research fellow for ASAP/OMSF with John D Chodera

- Science liaison for early-stage drug discovery for pandemic preparedness using artificial intelligence and free energy calculations for ASAP discovery.

University of Edinburgh & Cresset Group

2018-2022 / United Kingdom

PhD in Physical Chemistry with Julien Michel (Co-Sup: Mark Mackey & Antonia Mey)

- Applications of AI to AFE calculations in contemporary drug design. Advancing the field of free energy perturbation (FEP) with machine learning methodologies.

Cresset Group

2021 / United Kingdom

Doctoral research placement

- Dissection of softcore FEP algorithms to investigate optimisation of unreliable FEP transformations to push the boundaries of Flare software.

ModSim Pharma AB

2021-2022 / Sweden

Software development volunteer

- Open-source contributions to early-stage development of a browser-based FEP platform.

Université de Strasbourg

2018 / France

Research intern - group of Didier Rognan

- Molecular modelling and virtual screening of protein targets using advanced cavity detection and pharmacophore alignment algorithms.

Science Meets Business

2017-2019 / The Netherlands

Volunteer/ Chair

- Organising monthly networking events in the Leiden bioscience landscape; annual science-based start-up competitions.

Leiden University

2017-2018 / The Netherlands

Research intern - group of Ad IJzerman & Gerard van Westen

- *in silico* drug repurposing in triple negative breast cancer cell lines using chemogenomics-based virtual screening and *in vitro* hit validation.

Education

Leiden University

2012-2018

Bsc & Msc Bio-Pharmaceutical Sciences

- Drug Discovery oriented degree; emphasis on medicinal chemistry, ADME, toxicology and science-based business

Rotterdams Montessori Lyceum

2006-2012

Secondary school (Atheneum)

- STEM education with Pre-University honours programme (BPS)

Skills

Programming Languages	***Experienced:*** Python | Bash | LaTeX ***Familiar:*** Javascript
Frameworks & Libraries	Scikit-learn | Tensorflow | RDKit | Git | OpenMM | BioSimSpace | Slurm | SGE | Conda
Software Suites	Cresset | Schrödinger | GROMACS | Knime & PLP | Amber | ChemDraw | Sire | Adobe
Languages	***Native:*** Dutch ***Fluent:*** English ***Conversational:*** French, German

Awards & Publications

- Best Poster (AI-theme): 8th Annual CCPBioSim Conference 2022
- STEM for Britain 2022 finalist - presented research on FEP/ML in British House of Commons
- Best Talk: MGMS Young Modellers' Forum 2022
- Best Poster: 2nd RSC-BMCS / RSC-CICAG Artificial Intelligence in Chemistry 2020
- Best Poster: MGMS Young Modellers' Forum 2020/21
- Industrial Cooperative Awards in Science & Technology (iCASE)
- WSET Level 1/2/3 Award in Wines | Wine & Spirit Education Trust

[1] Antonia S. J. S. Mey, Bryce K. Allen, Hannah E. Bruce Macdonald, John D. Chodera, David F. Hahn, Maximilian Kuhn, Julien Michel, David L. Mobley, Levi N. Naden, Samarjeet Prasad, Andrea Rizzi, Jenke Scheen, Michael R. Shirts, Gary Tresadern, and Huafeng Xu. Best practices for alchemical free energy calculations [article v1.0]. *Living Journal of Computational Molecular Science*, 2(1):18378, 12 2020.

[2] Jenke Scheen, Mark Mackey, and Julien Michel. Data-driven generation of perturbation networks for relative binding free energy calculations. *ChemRxiv*, July 2022.

[3] Jenke Scheen, Wilson Wu, Antonia S. J. S. Mey, Paolo Tosco, Mark Mackey, and Julien Michel. Hybrid alchemical free energy/machine-learning methodology for the computation of hydration free energies. *Journal of Chemical Information and Modeling*, 60(11):5331–5339, 2020. PMID: 32639733.

[..] Currently two papers in preparation. Themes:

- An automated, open source, HPC-enabled RBFE pipeline using jupyter notebooks
- Benchmarking of a novel RBFE software