Jonathan Harrison

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https://github.com/shug3502

Scientific expertise

○ Machine Learning
○ Molecular Property Prediction
○ Drug Discovery
○ Bayesian Optimization/Active Learning
○ Bayesian Statistics

Education

2019. **DPhil in Systems Biology**
University of Oxford
Developing and applying modelling and Bayesian inference tools for cell biology
Supervised by Prof. R.E. Baker

2014. **MMath in Mathematics**
University of Oxford
1st class

Languages

Python	●●●	R	●●●
Julia	●●○	Stan	●●○
C++	●○○	Git	●●○

Current position

November 2024 – Present **Senior AI Research Scientist, Recursion**

July 2022 – October 2024 **AI Research Scientist, Exscientia**

The focus of my work is on molecular property prediction, including uncertainty quantification for machine learning models and with applications in Bayesian Optimization/Active Learning. I have experience leading a product team in this area.

I have developed strong software skills, taking projects from ideation to deployment and practical real world use. I have trained and fine-tuned foundation models for molecular property prediction. I am a core contributor to Molflux - a high profile open source ecosystem for machine learning for chemistry. Machine learning models and active learning software I have developed are used day-to-day by dozens of drug designers in their standard workflow.

Previous experience

Jan. 2019 – July 2022 **Postdoctoral Research Fellow, University of Warwick** (With Prof. N.J. Burroughs; Prof. A.D. McAinsh)

Using computational tools from Bayesian statistics, differential equations, stochastic modelling and image analysis, I provided insight into cell biology. I modelled chromosome dynamics allowing understanding of how and why cell division goes wrong. Conceptualized and supervised MSc rotation projects for 2 PhD students.

Jan. - Apr. 2018 **Data Science Intern at Hudl**

Worked within research and development team on a project investigating event detection in football matches using deep learning.

Selected Achievements, Presentations and Publications

Achieved 2nd place in public molecular property prediction competition run by Polaris **(2025)**

Recursion annual 10-K report included my analysis showing "a >2.5x increased efficiency in detecting new bioactive scaffolds with a >40% reduction in the flagging of likely cytotoxic compounds." **(2025)**

Invited talk at Active Learning in Pharma Symposium **(2024)**

O. Sen*, J.U. Harrison*, N.J. Burroughs, and A.D. McAinsh **(2021)** *Kinetochore life histories reveal the origins of chromosome mis-segregation and correction mechanisms* Developmental Cell https://doi.org/10.1016/j.devcel.2021.10.007 (All computational work - JUH, experiments - OS)

J.U. Harrison and R.E. Baker **(2020)** *An automatic adaptive method to combine summary statistics in approximate Bayesian computation* PLOS One https://doi.org/10.1371/journal.pone.0236954

For full list of publications see my Google Scholar profile