Arian Rokkum Jamasb

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Date of Birth: 5^{th} June 1996 | **Nationality:** Norwegian | **Webpage:** jamasb.io | **Github:** a-r-j | **LinkedIn:** /jamasb

Education

2018-(2022) *PhD.* **Computational Biology Group, Artificial Intelligence Group, Department of Computer Science and Biocomputing Group, Department of Biochemistry University of Cambridge**
Artificial intelligence for structural biology & drug discovery.
Supervisor: Professor Sir Tom Blundell, Department of Biochemistry.
Second Supervisor: Professor Pietro Lió, Department of Computer Science and Technology.

2014-2017 *BSc.* **Biochemistry, Imperial College London** (1^{st} Class Honours)
Dissertation: Automated Quantification of Cells Across Whole-Brain Image Volumes.
Specialist modules: Bioinformatics, Integrative Systems Biology, Neuroscience Research.

2007-2014 **The Perse School, Cambridge**. Academic Scholar.
A Levels: Mathematics, Further Mathematics, Biology, Chemistry

Research Experience

2021- *AI Resident.* **X - The Moonshot Factory (formerly Google[X])**, Mountain View, CA.

- Deep learning research for an early-stage project

2020-2021 *Machine Learning Consultant.* **Relation Therapeutics**, London, UK.

- Deep learning research for biological data

2017-2018 *Graduate Research Assistant.* ***Drosophila*** **Connectomics Group, Department of Zoology, University of Cambridge.** (Dr. G. Jefferis, Dr. M. Costa).
Neural Circuit Reconstruction and Connectomic Analysis of a Whole-Brain *Drosophila* Electron Microscopy Image Volume

- Examining odour information integration circuits and their role in innate sexual behaviour
- Neuroinformatics, development of computational tools, Analysis of electron micrographs
- Statistical image analysis, image registration

2017 *Undergraduate Dissertation.* Department of Life Sciences, Imperial College London. **Automated Quantification of Neuronal Distribution Across Whole-Brain Image Volumes** (Prof S. Brickley).

- Image processing, computer vision, algorithm design
- Whole-brain 2-photon imaging in mice
- Bioinformatics

2016-2017 *Undergraduate Research Assistant.* Department of Life Sciences, Imperial College London. **Developing a Dynamic Optogenetics System for High-Throughput Behavioural Manipulation of *Drosophila*** (Dr G. Gilestro).

- Statistical analysis and modelling of large time-series data
- Computer-aided design (CAD), 3D printing and electrical engineering
- Machine learning applied to behaviour analysis

Publications

Book Chapters

2021 **Deep Learning for Protein–Protein Interaction Site Prediction**.
A. R. Jamasb, B. Day, C. Cangea, P. Lió & T. L. Blundell. *Methods in Molecular Biology: Proteomics Data Analysis*. Springer.

Under Review

2021 **Structure-Aware Generation of Drug-Like Molecules.** P. Drotár, **A. R. Jamasb**, B. Day, C. Cangea, P. Lió. *Under review at MLSB 2021*

2021 **GrapHiC - A Python Library for Creating Bespoke Graph Datasets from Hi-C & Multi-omics Data**. D. Hall, **A. R. Jamasb**, M. Rozenwald, P. Lió. *Under Review at NeurIPS 2021*

2021 **A Case for Domain Expert Dataset Curation in Machine-Learning Enabled Chemistry.** R. Griffiths, A. R. Thawani, **A. R. Jamasb**, H. Moss, A. Bourached, P. Jones, W. McCorkindale, A. A. Aldrick. *Under Review at NeurIPS 2021*

2021 **Graphein - a Python Library for Geometric Deep Learning and Network Analysis on Protein Structures and Interaction Networks**. **A. R. Jamasb**, R. Viñas Torné, E. J. Ma, C. Harris, K. Huang, D. Hall, P. Lió, T. L. Blundell. *Under Review at NeurIPS 2021*

2020 **Message Passing Neural Processes** B. Day*, C. Cangea*, **A. R. Jamasb**, P. Lió. https://arxiv.org/abs/2009.13895. *Under Review at Journal of Machine Learning Research*

Pre-prints

2021 **On Graph Neural Network Ensembles for Large-Scale Molecular Property Prediction** E. E. Kosasih, J. Cabezas, X. Sumba, P. Bielak, K. Tagowski, K. Idanwekhai, B. A. Tjandra, **A. R. Jamasb**. https://arxiv.org/abs/2106.15529

2020 **The Photoswitch Dataset: A Molecular Machine Learning Benchmark for the Advancement of Synthetic Chemistry**
A. R. Thawani*, R. Griffiths*, **A. R. Jamasb**, A. Bourached, P. Jones, W. McCorkindale, A. Aldrick, A. A. Lee. https://arxiv.org/abs/2008.03226

Peer Reviewed

2021 **Predicted Structural Mimicry of Spike Receptor-Binding Motifs from Highly Pathogenic Human Coronaviruses.** C. A. Beaudoin, **A. R. Jamasb**, A. F. Alsulami, L. Copoiu, A. J. van Tonder, S. Hala, B. P. Bannerman, S. E Thomas, S. Chaitanya Vedithi, P. H M Torres, T. L. Blundell. *Computational and Structural Biotechnology Journal*

2021 **Utilising Graph Machine Learning within Drug Discovery and Development**
T. Gaudelet, B. Day, **A. R. Jamasb**, J. Soman, C. Regep, G. Liu, J. B. R. Hayter, R. Vickers, C. Roberts, J. Tang, D. Roblin, T. L. Blundell, M. M. Bronstein, J. P. Taylor-King. *Briefings in Bioinformatics.*

2020 **SARS-CoV-2-3D Database: Understanding the Coronavirus Proteome and Evaluating Possible Drug Targets**.
A. F. Alsulami*, S. Thomas*, **A. R. Jamasb***, C. Beaudoin, I. Moghul, B. Bannerman. L. Copoiu, S. C. Vedithi, P. Torres, T. L. Blundell. *Briefings in Bioinformatics*

2020 **Graphein - a Python Library for Geometric Deep Learning and Network Analysis on Protein Structures.**
A. R. Jamasb, P. Lió, T. L. Blundell. *Graph Representation Learning and Beyond Workshop at International Conference on Machine Learning (ICML) 2020*

2020 **Complete Connectomic Reconstruction of Olfactory Projection Neurons in the Fly Brain.**
A. S. Bates*, P. Schlegel*, R. J. V. Roberts, N. Drummond, I. F. M. Tamimi, R. G. Turnbull, X. Zhao, E. C. Marin, P. D. Popovici, S. Dhawan, **A. R. Jamasb**, A. Javier, F. Li, G. M. Rubin, S. Waddell, D. D. Bock, M. Costa, G. S. X. E. Jefferis. *Current Biology*

2020 **Benchmarking Scalable Active Learning Strategies on Molecules**
R. Griffiths, A. Aldrick, W. McCorkindale, P. Jones, **A. R. Jamasb**, B. J.Day, A. A. Lee. *Poster presented at Fundamental Science in the Era of AI Workshop at International Conference on Learning Representations (ICLR) 2020*

2019 **Functional and Anatomical Specificity in a Higher Olfactory Centre**
S. Frechter, A. S. Bates, S. Tootoonian, M. J. Dolan, J. D. Manton, **A. R. Jamasb**, J. Kohl, D. Bock, G. S. X. E. Jefferis. *eLife*

2017 **Ethoscopes: An Open Platform for High-Throughput Ethomics.**
Q. Geissmann, L. García Rodriguez, E. J. Beckwith, A. S. French, **A. R. Jamasb**, and G. F. Gilestro. *PLoS Biology.*

Scientific Computing and Programming[1]

`python` *Highly competent*: scientific computing, data analysis, machine learning, deep learning
`ML` *Highly Competent*: `PyTorch`, `Tensorflow`, `Keras`, `DGL`
`R` *Highly competent*: base functions, statistics, algebra, data visualisation and package development.
System *Competent*: GNU/Linux.
Web *Competent*: `javascript` and `HTML`/`CSS`.

Awards

2020 Fellow, Cambridge Philosophical Society (FCPS)
2020 Munro Studentship (teaching scholarship), *Queens' College, Cambridge*
2018 BBSRC PhD Studentship
2012-14 Chemistry Scholarship, *The Perse School, Cambridge*

Academic Service

Teaching & Supervision

Courses

2020 Part IA Discrete Mathematics
Department of Computer Science & Technology, University of Cambridge
2020 Part IB Artificial Intelligence
Department of Computer Science & Technology, University of Cambridge
2020 Part IB Computation Theory
Department of Computer Science & Technology, University of Cambridge
2019- Part II Computer Vision
Department of Computer Science & Technology, University of Cambridge
2019- Part II Bioinformatics
Department of Computer Science & Technology, University of Cambridge

[1] Most of my contributions are open-source and publicly available (see github.com/a-r-j)

MPhil Projects

2021 | *Structure-aware Generation of Molecules in Protein Pockets.* Pavol Drotar. (92%)

Undergraduate Projects

2021 | *Exploring Adversarial Attacks on Medical Image Trained Deep Neural Networks.* Melissa Yao (81%)

Reviewing

Journals | *Nature Machine Intelligence*
Computational and Structural Biotechnology
Journal of Open Source Software
Progress in Biophysics and Molecular Biology

Conferences | NeurIPS 2021

Workshops | *MLSys 21* Workshop on Graph Neural Networks and Systems (*GNNSys21*)
AAAI-21 Workshop on Graphs and more Complex Structures for Learning and Reasoning (*AAAI-21 GCLR*).
ML4Molecules Workshop at *NeurIPS 2020*
Graph Representation Learning and Beyond Workshop at *ICML 2020*

Volunteering and Outreach

2020 | Data Champion, Research Data Management Advocate, *University of Cambridge*
2019 | Local Organiser, *IWBDA Conference*
Events Officer, *Queens' College MCR*
2018 | Volunteer Demonstrator, Science Festival, *University of Cambridge*
2016 | Webmaster, *Imperial College Biochemistry Society*
Public engagement volunteer, *Biochemical Society*
Public engagement volunteer, *Royal Society of Biology.*
2014 | Volunteer tutor in mathematics, *Queen Edith's Primary School, Cambridge*

References

PhD Supervisor: Professor Sir Tom Blundell (tom@bioc.cryst.cam.ac.uk)
PhD Supervisor: Professor Pietro Lió (pl219@cam.ac.uk)
PI, Drosophila Connectomics Group: Dr Gregory Jefferis (jefferis@mrc-lmb.ac.uk)
Project Leader, Drosophila Connectomics Group: Dr Marta Costa (mmc46@cam.ac.uk)
Undergraduate Personal Tutor: Professor Anne Dell (a.dell@imperial.ac.uk)