# Arian Rokkum Jamasb

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Date of Birth: 5<sup>th</sup> June 1996 | Nationality: Norwegian | Webpage: jamasb.io | Github: a-r-j | LinkedIn: /jamasb

# **EDUCATION**

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 (1st 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.

## RESEARCH EXPERIENCE

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

A Levels: Mathematics, Further Mathematics, Biology, Chemistry

• Deep learning research for an early-stage project

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

• Deep learning research for biological data

Graduate Research Assistant. Drosophila Connectomics Group, Department of Zoology, Uni-2017-2018 versity 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
- 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

- 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
- 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.
- 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
- 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*.

## SELECTED TALKS

2021 | Artificial Intelligence in Drug Discovery. Astex Pharmaceuticals

# SCIENTIFIC COMPUTING AND PROGRAMMING<sup>1</sup>

- 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 AND AFFILIATIONS

2020	Fellow, Cambridge Philosophical Society (FCPS)
2020	Munro Studentship (teaching scholarship), Queens' College, Cambridge
2018	BBSRC PhD Studentship
2017	Associate, Royal College of Science (ARCS)

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

 $<sup>^1\</sup>mathrm{Most}$  of my contributions are open-source and publicly available (see <code>github.com/a-r-j)</code>

	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

#### 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
Briefings in Bioinformatics
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

### 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

Graph Representation Learning and Beyond Workshop at ICML 2020

# LINKS

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Webpage jamasb.io

GitHub github.com/a-r-j

LinkedIn linkedin.com/in/jamasb

Google Scholar

Semantic Scholar

ResearchGate https://www.researchgate.net/profile/Arian-Jamasb
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# REFERENCES

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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)
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