# 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**

2018-(2022)	<ul> <li>PhD. Computational Biology Group, Artificial Intelligence Group, Department of Computer Science and Biocomputing Group, Department of Biochemistry University of Cambridge</li> <li>Artificial intelligence for structural biology &amp; drug discovery.</li> <li>Supervisor: Professor Sir Tom Blundell FRS, Department of Biochemistry.</li> <li>Second Supervisor: Professor Pietro Lió, Department of Computer Science and Technology.</li> </ul>
2014-2017	BSc. Biochemistry, Imperial College London (1 <sup>st</sup> 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-	Visiting PhD Student. Laboratory of Protein Design & Immunoengineering, EPFL (Prof Bruno Correia) Lausanne, CH.
2021	Research Intern. MILA - Montreal Institute for Learning Algorithms (Prof Jian Tang), Montreal, Canada.
2021	AI Resident. X - The Moonshot Factory (formerly Google[X]), Mountain View, CA.
2020-2021	Machine Learning Consultant. Relation Therapeutics, London, UK.
2017-2018	Graduate Research Assistant. Drosophila Connectomics Group, Department of Zoology, University of Cambridge. (Dr. G. Jefferis, Dr. M. Costa). Cambridge, UK Neural Circuit Reconstruction and Connectomic Analysis of a Whole-Brain Drosophila Electron Microscopy Image Volume
	<ul> <li>Examining odour information integration circuits and their role in innate sexual behaviour</li> <li>Neuroinformatics, development of computational tools, Analysis of electron micrographs</li> </ul>

- 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 Structural Characterization of Newly Discovered ORFs in the SARS-CoV-2 Proteome. C. A. Beaudoin\*, A. F. Alsulami\*, L. Copoiu\*, A. R. Jamasb\*, S. C. Vedithi, P. H.M. Torres, T. L. Blundell. *Under review*.
- 2020 Message Passing Neural Processes B. Day\*, C. Cangea\*, A. R. Jamasb, P. Lió. https://arxiv.org/abs/2009.13895. *Under Review*.

#### PRE-PRINTS

- 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.
- 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.
- 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. bioRxiv
- 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

- 2021 Structure-Aware Generation of Drug-Like Molecules. P. Drotár, A. R. Jamasb, B. Day, C. Cangea, P. Lió. NeurIPS-W MLSB 2021 (Selected for spotlight talk)
- 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
2021 ELIXIR 3D BioInfo Community Annual Meeting 2021. Poster
2020 Graph Representation Learning and Beyond Workshop at ICML (ICML-GRL+). Poster

# 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.

## **Projects**

Graphein - open source library for constructing geometric representations of biological data.

Protein Viewer - VSCode extension for viewing protein structures in the editor

## AWARDS AND AFFILIATIONS

Perry Award, Queens' College, Cambridge
President's Letter for Outstanding Academic Achievement, Queens' College, Cambridge
Fellow, Cambridge Philosophical Society (FCPS)
Munro Studentship (teaching scholarship), Queens' College, Cambridge
BBSRC PhD Studentship
Associate, Royal College of Science (ARCS)
Chemistry Scholarship, The Perse School, Cambridge

<sup>&</sup>lt;sup>1</sup>Most of my contributions are open-source and publicly available (see github.com/a-r-j)

## ACADEMIC SERVICE

#### TEACHING & SUPERVISION

#### Courses

2020	Part IA Discrete Mathematics
	Department of Computer Science & Technology, University of Cambridge
2020	Part IB Artificial Intelligence
	$Department\ of\ Computer\ Science\ \mathscr{C}\ Technology,\ University\ of\ Cambridge$
2020	Part IB Computation Theory
	$Department\ of\ Computer\ Science\ \mathscr{C}\ Technology,\ University\ of\ Cambridge$
2019-	Part II Computer Vision
	$Department\ of\ Computer\ Science\ \mathscr{C}\ Technology,\ University\ of\ Cambridge$
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%). Selected for oral presentation at NeurIPS-MLSB.

#### Undergraduate Projects

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

#### REVIEWING

Journals

Nature Machine Intelligence

IEEE/ACM Transactions on Computational Biology and Bioinformatics

Briefings in Bioinformatics

Computational and Structural Biotechnology

Journal of Open Source Software

Progress in Biophysics and Molecular Biology

Conferences NeurIPS 2021

Workshops

AAAI-22 Workshop on Graphs and more Complex structures for Learning and Reasoning (AAAI-22

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

## 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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