

MIGUEL GARCIA-ORTEGON

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EDUCATION

- **PhD in Probabilistic Machine Learning for Molecules** Oct 2019 – Mar 2024
University of Cambridge (Cambridge, UK)
Supervised by Sergio Bacallado, Andreas Bender and Carl Rasmussen. Working on meta-learning, antibiotic screening, model benchmarking, molecular optimization. Using VAEs, Bayes Opt, graph NNs, neural processes.
- **MRes in Mathematical Genomics and Medicine** Oct 2018 – Sep 2019
University of Cambridge (Cambridge, UK). Score 70%.
- **MSc in Mathematical Engineering** Sep 2017 – Jun 2018
Universitat Politècnica de Catalunya (Barcelona, Spain). Score 90%.
- **MPhil in Scientific Computing** Oct 2015 – Sep 2016
University of Cambridge (Cambridge, UK). Score 74%.
- **BSc in Biotechnology (4-year degree)** Sep 2011 - Jul 2015
Universidad Pablo de Olavide (Sevilla, Spain). Score 96%.

EXPERIENCE

- **Machine learning scientist.** *Novo Nordisk* (London, UK) Dec 2023 – Ongoing
Sequence representation learning for therapeutic peptides and small proteins.
- **Research intern.** *Microsoft Research Cambridge* (Cambridge, UK) May 2022 – Jul 2022
Generative modelling of T-cell receptor repertoires.
- **Teaching assistant.** *Engineering Dept, University of Cambridge* (Cambridge, UK) Jan 2020 – Mar 2020
Supervision of 4 third-year undergraduate students for the module 3F8 Inference.
- **Research assistant.** *EMBL - Centre for Genomic Regulation (CRG)* (Barcelona, Spain) Feb 2018 – Sep 2018
Development of cancer diagnostics with SVMs using transcriptomic data.
- **Deep learning intern.** *Partium (formerly Catchoom)* (Barcelona, Spain) Oct 2017 – Dec 2017
Transfer learning of residual CNNs originally trained on ImageNet.
- **Research intern.** *MRC Laboratory of Molecular Biology (LMB)* (Cambridge, UK) Jun 2014 – Sep 2014
Structural studies of an autophagosome protein.

PUBLICATIONS

- **M Garcia-Ortegon**, A Bender, C Rasmussen, S Bacallado. A transfer learning approach to antibacterial screening of ultra-large chemical libraries. *In preparation*.
- **M Garcia-Ortegon**, S Seal, A Bender, C Rasmussen, S Bacallado. Graph neural processes for molecules: Benchmarking on docking scores reveals simple strategies to improve meta-generalization. *Submitted*.
- D Cagnina, **M Garcia-Ortegon**, MR Costa-Jussa, L Mazzearella, M Weber, L Serrano, MH Schaefer. Tissue-of-origin prediction of different onco-types from gene expression profiles. *Submitted*.
- S Seal, O Spjuth, L Hosseini-Gerami, **M Garcia-Ortegon**, S Singh, A Bender, A Carpenter. Insights into drug cardiotoxicity from biological and chemical data: The first public classifiers for FDA DICTrank. *Accepted at JCIIM*.

- **M Garcia-Ortegon**, A Bender, S Bacallado. Conditional neural processes for molecules. In *Machine Learning for Structural Biology Workshop*, and *Meta-Learning Workshop, NeurIPS* (2022).
- **M Garcia-Ortegon**, GNC Simm, AJ Tripp, JM Hernandez-Lobato, A Bender, S Bacallado. DOCKSTRING: easy molecular docking yields better benchmarks for ligand design. In *JCIM* (2022).
- M Thomas, A Boardman*, **M Garcia-Ortegon***, H Yang, C Graaf, A Bender. Applications of artificial intelligence in drug design: opportunities and challenges. In the book *Artificial Intelligence in Drug Design*, (2022).
- RR Griffiths, AA Aldrick, **M Garcia-Ortegon**, V Lalchand, AA Lee. Achieving robustness to aleatoric uncertainty with heteroscedastic Bayesian optimisation. In *Machine Learning: Science and Technology* (2021).
- **M Garcia-Ortegon**, A Bender, CE Rasmussen, H Kajino, S Bacallado. Combining variational autoencoder representations with structural descriptors improves prediction of docking scores. In *Machine Learning for Structural Biology Workshop*, and *Machine Learning for Molecules Workshop, NeurIPS* (2020).
- RR Griffiths, AA Aldrick, **M Garcia-Ortegon**, AA Lee. Heteroscedastic Bayesian optimisation in scientific discovery. In *Machine Learning and the Physical Sciences Workshop, NeurIPS* (2019).
- Y Ohashi, N Soler, **M Garcia-Ortegon**, L Zhang, ML Kirsten, O Perisic, GR Masson, JE Burke, AJ Jakobi, AA Apostolakis, CM Johnson, M Ohashi, N Ktistakis, C Sachse, RL Williams. Characterization of Atg38 and NRBF2, a fifth subunit of the autophagic Vps34/PIK3C3 complex. In *Autophagy* (2016).

AWARDS

- **Wellcome Trust MRes+PhD Scholarship** Oct 2018 – Ongoing
Full funding for MRes and PhD fees, stipend and research expenses. Worth £165,000.
- **Best Poster Prize at the 4th MABC Conference** Jul 2021
Most voted poster in the 4th ML and AI in Bio(Chemical) Engineering Conference (MABC).
- **'la Caixa' Bank Postgraduate Scholarship.** Oct 2015 – Sep 2016
Full funding for MPhil fees and stipend. Worth £24,000.
- **Wolfson College Studentship.** Oct 2015
Awarded to outstanding incoming Wolfson students. Worth £2,000.
- **Spanish Research Council Scholarship** Feb 2014
Awarded to outstanding undergraduates to do research in a Spanish laboratory. Worth £2,000.
- **LMB Summer Studentship** Jun 2014 – Sep 2014
Awarded to outstanding undergraduates to do research in the LMB, Cambridge. Worth £5,000.
- **Atlanticus-Santander Mobility Scholarship** Sep 2013 - Dec 2013
Awarded to outstanding undergraduates at Universidad Pablo de Olavide to study at a North American or Australian university.

SKILLS

- **Python:** PyTorch, numpy, matplotlib, scikit-learn, pandas, DeepChem.
- **Workflow:** Vim, i3wm, Git, bash, GNU/Linux, L^AT_EX, VS Code.
- **Languages:** English (proficient), Spanish (native).

REFERENCES

Available upon request.