CURRICULUM VITAE JOSEPH WALLACE

PERSONAL INFORMATION

Family Name, First Name: Wallace, Joseph
Date and place of Birth: 22/09/1995, Auckland, New Zealand
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EDUCATION

09/2017-06/2022 **PhD Computational Biochemistry**, University of Liverpool, UK. Thesis Title: "How does constraining folded peptides within a dense self-assembled monolayer on gold nanoparticles affect their structure?" Supervisors: Prof Raphael Levy, Dr Michael Sullivan, Dr Martin Volk.

09/2014-06/2017 **BSc. Biochemistry (Hons)**, First Class, University of Liverpool, UK. Project: "Solving the crystal structure of Cytochrome BC1 for the development of antimalarial drugs."

RESEARCH EXPERIENCE

01/2023- Present **Postdoc Researcher,** Istituto Italiano di Tecnologia, Genova, Italy. Development of a screening pipeline based on simulation and machine learning algorithms for the prediction of small molecule binding to nanoparticles.

12/2022-12/2023 **Postdoc Researcher,** Università degli studi di Padova, Padova, Italy. Utilise computational methods, such as simulation and machine learning, for the further development and understanding of nanoparticle-based receptors.

09/2021 – 05/2022 **Research Attachment,** Université Sorbonne Paris Nord (Paris 13), France. Aid in the relocation of the lab, including facilitating new local research networks while utilising simulations to understand self-assembled monolayers on gold.

04/2019 – 04/2021 **Research Attachment**, Institute of High-Performance Computing, A*STAR, SG. Computational methods such as enhanced sampling molecular dynamics simulations for understanding self-assembled monolayer formation.

06/2016 – 08/2016 **Summer Studentship**, Wellcome Trust Funded, University of Liverpool, UK Aimed at investigating potential non-heparin anticoagulants with antithrombin.

TECHNICAL SKILLS AND COMPETENCES

Molecular dynamics simulations of nanoparticle systems utilising a variety of methods such as enhanced sampling methods (HREMD, SteeredMD, Umbrella Sampling, MetaD) for free energy calculations. Strong coding skills in Python alongside comfort in high-performance Linux-based systems. Computational Programs: GROAMCS, PLUMED, Python (TensorFlow/Keras, PyTorch), Git/Github.

PUBLICATIONS

Franco-Ulloa, S., Cesari, A., Riccardi, L., Wallace, J., Mancin, F., De Vivo M. High-throughput In-Silico Screening of Nanoparticle-based Supramolecular Hosts. In Prep.