

Simon CROUZET

LOOKING FOR ML RESEARCH ENGINEER POSITIONS IN DRUG DISCOVERY



Work Experiences

2023 - 2025

Research Scientist - EPFL (Switzerland)

Development of a conditional diffusion model based on RFDiffusion to sample antibody backbone decoys. Conception of a sequence-structure guided codesign pipeline for antibody discovery based on AlphaFold and ProteinMPNN, using cryoEM density maps. Deployment of diverse tools to build and refine protein structures from cryoEM data and to evaluate protein-protein binding conformations based on Rosetta. Deployment of MD simulations using GROMACS to study viral capsid variants.

2022 Computational Biologist Intern - Roche (Switzerland)

Design and development of a knowledge graph neural network (GNN) method, called *G-PLIP*, for protein ligand bioactivity prediction. Analysis of data generated by phenotypic screens and identification of putative high-potential targets for novel drug discovery programmes using explainable AI.

2022 Research Assistant - ETH Zurich (Switzerland)

Design, implementation, and evaluation of a recurrent neural network (RNN) to predict HIV evolutionary pathways, induced drug resistance and designing optimal treatment combinations.

2021 Research Assistant - Wellcome Sanger Institute (England)

Pangenomics exploration of *Anopheles Funestus* (mosquito, major vector of malaria). Development of a SnakeMake pipeline for the characterization and analysis of short and long-range structural variation events from high-quality assemblies of specimens.

2020 Research Intern - University of Glasgow (Scotland)

Development and improvement of a viral host prediction model in Julia through genomic feature, phylogenetic neighbourhoods (using BLAST search) and protein characteristics.

2018 Research Intern - Aix-Marseille University (France)

Development in C of an automaton network solver using data-flow algorithms to model genetic regulatory networks as the control of floral morphogenesis in *Arabidopsis Thaliana*.



Qualifications

2021 - 2022

M.Sc. in Systems biology, Genomics and Bioinformatics - *with First Class Honours*
Ecole Normale Supérieure (ENS-PSL) - Paris (France)

2020 - 2021

M.Sc. in Bioinformatics and Modelling - *with High Honours*
Sorbonne University - Paris (France)

2019

Semester Abroad during B.Sc. in Computer Science
Linnaeus University - Växjö (Sweden)

2017 - 2020

B.Sc. in Computer Sciences - *with First Class Honours*
Aix-Marseille University - Marseille (France)

2016 - 2017

Interruption of studies due to health issues

2013 - 2016

B.Sc. in Chemistry
Grenoble Alpes University - Grenoble (France)



Achievements & Awards

Publications available on [Google Scholar](#)

2024 "AI For Good" Hackathon Winner - *Entrepreneur First*

2022 IP2TIS "Think Tank in Innovation & Sustainability" Fellow - *Roche Holding Ltd.*

2021 Qlife Institute Scholarship - *École Normale Supérieure (ENS-PSL)*

2018 FIP « Incubateur de Jeunes Talents » Scholarship - *Aix-Marseille University*



Contact & Info

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Nationality: French

(Work Permit: B)



Skills

Programming:

Languages:

Main: Julia, Python

Others: R, Java, C, C++, SQL, Matlab, PHP, HTML/CSS,

Fields of Interest:

Artificial Intelligence, Machine Learning, Deep Learning, Neural Networks, Computational Biology, Drug Discovery, Protein Design, Precision Medicine, Genomics, Systems Modelling, Problem Solving

OS:

Windows, GNU/Linux

Tools:

Git, Unit Testing, Object Oriented Programming, Parallel Programming, HPC Cluster, PowerBI

Libraries:

PyTorch, PyTorch-Geometric, TensorFlow, JAX, Rosetta, Rfdiffusion, ProteinMPNN, AlphaFold, ColabDesign, ...

Transversal:

Project Management



Languages

French: Native

English: Fluent

TOEFL iBT (04.2020): 99/120