Vincent Mallet

Researcher, CBIO, Mines Paris

Research Experience

2024 - **Tenure-track researcher**, *CBIO - Mines Paris*, Paris
Finding the right representation for learning on RNA and protein structures
Finding how to go beyond static structures with cryo-EM and how to use conformations in machine learning applications
Applying those findings to structural bioinformatics and drug design

2023 - 2024 **Postdoctoral researcher**, *LIX in Polytechnique / Sanofi*, Paris
Supervised by Maks Ovsjanikov
Geometric learning methods for proteins: Compare protein structure representations and how they can be combined.
Finding antibodies in cryo-EM densities: Partnership with Sanofi to use object detection to automatically identify antibodies in cryo-EM maps.

2022 **Visiting Student**, *La Sapienza Gladia Group*, Rome
Supervised by Emanuele Rodolà
Surface methods for proteins: Adapt latest surface methods to learning on protein surfaces.

2019 - 2022 **PhD Candidate**, *Structural Bioinformatics, Institut Pasteur / CBIO, Mines Paris*, Paris
Supervised by Michael Nilges and Jean-Philippe Vert.
Reinforcement learning and cryo-EM: Train an agent to trace protein backbones in cryo-EM densities.
Equivariant networks for genomic data: Create a theoretical framework that encompasses existing methods. Implement it and get enhanced results.
Assist Protein-Protein Interaction drug design: Develop the first binding pocket predictor for this data.
Learning on RNA structure as 2.5D graphs: Develop a library for this representation, relevant deep learning layers and motifs mining algorithms.

2018 - 2019 **Master Thesis**, *McGill Computational Biology Group*, Montréal
Supervised by Jérome Waldispühl.
Active ligand generation project: Condition the generation of small molecules on the structure of a protein pocket.
RNA structural drug design: Represent binding pockets as 2.5D graphs and use machine learning to predict active compounds from it.

Spring 2018 **Research Internship**, *McGill Computational Biology Group*, Montréal
Developed binding site comparison and embedding for proteins based on graphs vs spatial point sets.

Education

2018 - 2019 **M.Sc. Computer Science**, *McGill University*, Machine Learning, Deep Learning, Bioinformatics

2015 - 2018 **M.Eng. Bioinformatics**, *Ecole Polytechnique*, Parallel computing, Big Data, Machine Learning, Bioinformatics

2013 - 2015 **Preparatory Program**, *Louis le Grand*, PCSI/PC Track

Teaching

2022-23-24 **Teacher**, *CRI (Centre de Recherche Interdisciplinaire)*, 30 hours of classes and practical sessions on Foundations of AI. Joined the board of teachers.

2022 **Lecturer**, *McGill CS Master*, Geometric learning for drug design

2020-21-22 **Lecturer**, *Université de Paris, Master ISDD*, Generative models for drug design

Publications

Journals

2023 ▷ **Alignscape, displaying sequence similarity using self-organizing maps**. Isaac Filella-Merce, Vincent Mallet, Eric Durand, Michael Nilges, Guillaume Bouvier, and Riccardo Pellarin. *Frontiers in Bioinformatics*, 4, 2024

2022 ▷ **InDeep: 3D fully convolutional neural networks to assist in silico drug design on protein-protein interactions**. Vincent Mallet, Luis Checa Ruano, Alexandra Moine Franel, Michael Nilges, Karen Druart, Guillaume Bouvier, and Olivier Sperandio. *Bioinformatics*, 2022

2022 ▷ **RNAglib: A python package for RNA 2.5D graphs**. Vincent Mallet, Carlos Oliver, Jonathan Broadbent, William L Hamilton, and Jérôme Waldispühl. *Bioinformatics*, 2022

2022 ▷ **VeRNAl: A Tool for Mining Fuzzy Network Motifs in RNA**. Carlos Oliver*, Vincent Mallet*, Pericles Philippopoulos, William L Hamilton, and Jérôme Waldispühl. *Bioinformatics*, 2022

2021 ▷ **quicksom: Self-Organizing Maps on GPUs for clustering of molecular dynamics trajectories**. Vincent Mallet, Michael Nilges, and Guillaume Bouvier. *Bioinformatics*, 2021

2020 ▷ **OptiMol: Optimization of binding affinities in chemical space for drug discovery**. Jacques Boitreaud*, Vincent Mallet*, Carlos Oliver, and Jérome Waldispuhl. *Journal of Chemical Information and Modeling*, 2020

2020 ▷ **Augmented base pairing networks encode RNA-small molecule binding preferences**. Carlos Oliver, Vincent Mallet, Roman Sarrazin Gendron, Vladimir Reinharz, William L Hamilton, Nicolas Moitessier, and Jérome Waldispuhl. *Nucleic Acids Research*, 2020

Conferences

2021 ▷ **Reverse-complement equivariant networks for dna sequences**. Vincent Mallet and Jean-Philippe Vert. *Advances in Neural Information Processing Systems*, 2021

Preprints

2023 ▷ **Finding antibodies in cryo-em densities with crai**. Vincent Mallet, Chiara Rapisarda, Hervé Minoux, and Maks Ovsjanikov. *bioRxiv*, 2023. 10.1101/2023.09.27.559736

2023 ▷ **Structure-based rna drug discovery with deep-learning assisted virtual screening**. Juan Guillermo Carvajal Patiño, David Becerra, Vincent Mallet, David Hiraki, Nicolas Moitessier, Luis Fernando Niño, Carlos Oliver, and Jérôme Waldispühl. *(In preparation)*, 2023

2023 ▷ **Atomsurf : Surface representation for learning on protein structures**. Vincent Mallet, Souhaib Attaiki, and Maks Ovsjanikov. *arXiv preprint arXiv:2309.16519*, 2023

2023 ▷ **Approximate network motif mining via graph learning**. Carlos Oliver, Dexiong Chen, Vincent Mallet, Pericles Philippopoulos, and Karsten Borgwardt. *arXiv preprint arXiv:2206.01008*, 2023

2022 ▷ **Edge-similarity-aware graph neural networks**. Vincent Mallet, Carlos G Oliver, and William L Hamilton. *arXiv preprint arXiv:2109.09432*, 2021

2019 ▷ **Leveraging binding-site structure for drug discovery with point-cloud methods**. Vincent Mallet, Carlos G Oliver, Nicolas Moitessier, and Jerome Waldispuhl. *arXiv preprint arXiv:1905.12033*, 2019

Talks

2023 **Modeling structural biology with geometric deep learning** , *Data Shapes Seminar, INRIA Paris*

2023 **Geometric learning for drug design**, *AstraZeneca drug discovery Seminar (online)*

2023 `RNAGlib`**: a platform for learning on RNA structure**, *MILA drug discovery Seminar*

2023 **Reverse-Complement Equivariant Networks for DNA Sequences** , *20 min talk, AI in Structural Biology Workshop*

2022 **InDeep: learning for drug design on protein protein interactions** , *Workshop on AI in magnetic resonance*

2022 **Artificial Intelligence in prediction, determination and analysis of structures**, *EMBO workshop: Machine learning for structural biology*

2022 **Reverse-Complement Equivariant Networks for DNA Sequences**, *NeurIPS*

Funding

2022 ELISE Mobility Award
2019 PhD funding from the INCEPTION Program
2019 Granted AMX PhD funding
2018 Research Grant from the Computational Biology Group

Publishing

`Reviewer`: Bioinformatics, NAR, NeurIPS, ICML
`Associate Editor`: Frontiers in Bioinformatics

Technical Skills

`Libraries`: Deep learning (PyTorch, DGL, Keras, TensorFlow, Sonnet, JAX, Haiku), Bioinformatics (Chimerax, Biopython, RDKit, Pymol)
`Developed packages`: `rnaglib`, `quicksom`

Languages

French: Native, English: Fluent (TOEFL 117), German, Italian:(Intermediate)

Additional Interests

Scenography In charge of scenography for `Phasm`, an association organizing festivals and concerts.
Sports Climbing, Running, Fencing, Skiing