Vincent Mallet

Tenure-track Researcher · Ecole des Mines

60, Boulevard Saint-Michel, Paris, France, 75006

vincent.mallet@minesparis.psl.eu | vincentx15.github.io | Vincentx15

Curriculum

2024 -	**Tenure-track researcher**, CBIO - Mines Paris
2023 - 2024	**Postdoctoral researcher Supervised by Maks Ovsjanikov**, Ecole Polytechnique
2022	**Visiting Student with Emanuele Rodolà**, La Sapienza
2019 - 2022	**PhD supervised by Michael Nilges and Jean-Philippe Vert**, Institut Pasteur / Mines Paris
2018 - 2019	**MSc in Computer Science with Jérôme Waldispühl**, McGill Computational Biology Group
2013 - 2019	**MSc in Bioinformatics**, Ecole Polytechnique

Publications

Journals

Structure-based rna drug discovery with deep-learning assisted virtual screening. Juan Guillermo Carvajal Patiño*, Vincent Mallet*, David Becerra, Luis Fernando Niño, Carlos Oliver, and Jérôme Waldispühl. *Nature Communications*, 2025

Indeepnet: a web platform for predicting functional binding sites in proteins using indeep. Fabien Mareuil, Rachel Torchet, Luis Checa Ruano, Vincent Mallet, Michael Nilges, Guillaume Bouvier, and Olivier Sperandio. *Nucleic Acids Research*, page gkaf403, 2025

Finding antibodies in cryo-em maps with crai. Vincent Mallet, Chiara Rapisarda, Hervé Minoux, and Maks Ovsjanikov. *Bioinformatics*, 41(5):btaf157, 2025

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

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

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

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

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

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

Luis Wyss, Vincent Mallet, Wissam Karroucha, Karsten Borgwardt, and Carlos Oliver. A comprehensive library for rna structure-function modeling. In *ICLR 2025 Workshop on AI for Nucleic Acids*

Atomsurf : Surface representation for learning on protein structures. Vincent Mallet*, Souhaib Attaiki*, Yangyang Miao*, Bruno Correia, and Maks Ovsjanikov. *ICLR*, 2025

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

Awards, Fellowships, & Grants

2025 **PSL PhD Fellowships for Victor Gertner**,
2024 **3 PhD Fellowships for Wissam Karroucha**, FRM, PSL, ITN Mines
2022 **Elise Mobility Award**, ELLIS
2019 **2 PhD Fellowship**, INCEPTION Program, AMX

Presentations

2025. *Machine learning on the structure of biomolecules*. GT Masim, Paris.

2025. *Machine learning on the structure of biomolecules*. CBS Montpellier.

2024. *Learning on protein structures*. Bits in Bio Paris.

2024. *Learning on protein structures, with applications in Cryo-EM*. Pasteur Symposium on AI.

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*. AI in Structural Biology Workshop.

2022. *Representation learning on the structure of biomolecules* GT MASIM, Paris

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.

Teaching Experience

2025 **Lecturer**, *Ecole des Mines* Modern drug design with learning approaches
2022-2024 **Teacher**, *CRI Paris* 45 hours of classes and practical sessions on Foundations of AI
2022 **Lecturer**, *McGill CS Master* Geometric learning for drug design
2020-2022 **Lecturer**, *Université de Paris, Master ISDD* Generative models for drug design

Mentoring

Supervisions

2025- **Victor Gertner**, PhD Student
2025- **Nicolas Portal**, Post-Doc
2025- **Ikram Mahmoudi**, Post-Doc
2025- **Wissam Karroucha**, PhD student
2025- **Victor Laigle**, PhD student

Co-supervisions

2024- **Tian Zhu**, PhD student, *with Bruno Correia, EPFL*
2024- **Mrunali Manjrekar**, PhD student, *with Maz Abulnaga, MIT*
2024- **Yangyang Miao**, PhD student, *with Bruno Correia, EPFL*
2024- **Tamara Künzle**, PhD student, *with Maks Ovsjanikov, Ecole Polytechnique*
2022 **Jacques Boitreaud**, Msc student, *with Jérôme Waldispühl, McGill*

Additional involvements

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

Organizing member: CNRS GT Masim
Developed packages: `rnaglib`, `quicksom`, `CrAI`, `RNAmigos2`