

Lorenzo Di Fruscia

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EDUCATION

Delft University of Technology

PhD candidate, **Pattern Recognition & Bioinformatics**

Feb, 2024 – Present

Delft, The Netherlands

- Molecular representation learning, multimodal learning, large language models, generative modeling.

Sapienza University

Master's degree, Physics

Nov, 2019 - Sep, 2022

Rome, Italy

- Final grade: **110/110**
- GPA: **3.92/4.00**
- Thesis: Development of a human respiratory model with graph-based Geometric deep learning methods
- Main courses: Deep learning and artificial intelligence, physics of complex systems, soft and biological matter, physics of liquids, theory of stochastic processes, statistical mechanics and critical phenomena.

Sapienza University

Bachelor's degree, Physics

Nov, 2016 - Nov, 2019

Rome, Italy

- Final grade: **110/110**
- GPA: **3.67/4.00**
- Thesis: Markovian and stochastic processes: derivation and applications

EXPERIENCE

National Research Council of Italy (CNR)

Scientific collaborator at **Institute for applied mathematics (IAC)**

Dec, 2022 – Dec, 2023

Rome, Italy

- Geometric deep learning (graphs, point clouds), computational fluid dynamics, and explainable AI (XAI)

MedLea Srls

Deep learning specialist

Dec, 2022 – Dec, 2023

Rome, Italy

- Designing artificial intelligence algorithms for respiratory diagnosis and prognosis

PUBLICATIONS

1. [Leveraging large language models for enzymatic reaction prediction and characterization](#)
L Di Fruscia, J.M. Weber. Digital Discovery 4 (12), **2025**
2. [Grounding Large Language Models in Reaction Knowledge Graphs for Synthesis Retrieval](#)
O. Bunkova, L. Di Fruscia, S. Rupprecht, A.M. Schweidtmann, M.J.T. Reinders, J.M. Weber.
ML4Molecules, ELLIS UnConference, **2025**

INVITED TALKS

- [Graphs & Data](#) seminar, Feb 2026 Delft

CONFERENCES, SYMPOSIA AND SCHOOLS

- From Graph Neural Networks to Explainable AI [School](#)
 - BioSB Conference, [Poster](#)
 - OxML Representation Learning, [School](#)
- Liverpool, Sep, 2023
Egmond aan Zee, June 2024
Oxford, July 2024

- Generative Modeling Summer [School](#) (GEMSS)
- Statlearn Workshop, [Poster](#)
- AI4Bio symposium, [Poster](#)
- ELLIS ML4Molecules, [Poster](#)
- AI4Bio symposium, [Poster](#)

Antibes, Apr 2025
Antibes, Apr 2025
Delft, Apr 2025
Copenhagen, Dec 2025
Delft, Apr 2026

TEACHING

- Supervised **4** Master's students (*Feb 2024–Present*)
- Recent Topics in Bioinformatics (MSc, 2024)
- Bioinformatics, Data Analysis (BSc, 2025)
- Bioinformatics, Data Analysis (BSc, 2026)

SERVICE

- [AI4Bio symposium](#), organizer (Apr, 2026)
- [AI4Bio webinar](#), host (Apr, 2026)

SKILLS

- **Skills:** Python (NumPy, PyTorch, PyTorch Geometric, PyTorch Lightning), Git, Linux, Docker, C++.
- **Languages:** Italian (mother tongue), English (advanced)