



UNIVERSITÀ POLITECNICA DELLE MARCHE

Supervisor: Dr. Giovanni Di Muccio

Dept. of Life and Environmental Sciences



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**Computational Biology for Molecular Recognition
and Next-Generation Biosensing Technologies**



Role: Young Researcher (RTD-A) in Molecular Biology and Lecturer in Structural Bioinformatics; Head of the Computational Unit of the Mollab@NY-MaSBiC group. Expert in the field of Computational NanoBiotechnology, in particular **Nanopore sensing, Molecular Dynamics** simulations, and enhanced **Free-Energy** based sampling techniques.

Previous experiences

Postdoc PNRR National Biodiversity Center (NBFC) at UNIVPM, on the design and development of **graphene based biosensors** for **estradiol detection** at ultra-low concentrations.

ERC-funded postdoctoral researcher in the HyGate project at Sapienza University of Rome, where he investigated the **gating and selectivity** mechanisms of **biological and artificial nanopores** and contributed to the development of memristive nanopore platforms for **neuromorphic applications**.

Author of more than 20 peer-reviewed publications in international journals, including Advanced Materials, ACS Nano, Nature Communications, JACS, PNAS, Small Methods, and involved in several international collaborations on nanopore sensing, molecular simulations, and biomolecular modelling for medical and environmental application

Supervision and mentoring

3 PhD student (1 ongoing), 7 Master students (4 ongoing)

H-index 9, ORCID: <https://orcid.org/0000-0003-1388-8806>

Principal investigator of **High Performance Computing** projects focused on the computational investigation of nanopore systems and biomolecular interactions:

- **SLIGHT** – EuroHPC Extreme Scale Access (MareNostrum5, 2024).
- **NOVOBAR** – CINECA IS CRA-B (Leonardo, 2023).

Research Projects and Collaborations

- Design of peptidic inhibitors targeting cancer and neurodegenerative molecular pathways (collaboration with Istituto Nazionale dei Tumori and University of Milan).
- Investigation of protein detection in biological nanopores, in collaboration with international research groups (Groningen, DTU, Uppsala, Columbia).





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THE RESEARCH GROUP: MoLab@NY-MaSBiC

The **Molecular Biology Laboratory MoLab** is a research group working at the interface between **molecular biology, computational biology, and biotechnology**.

The laboratory is part of the **New York - Marche Structural Biology Center (NY-MaSBiC)** and collaborates with several research groups in structural biology, computational biophysics, and nanobiotechnology.

The group integrates **experimental and computational approaches** to investigate biomolecular systems, molecular recognition processes, and the development of innovative biosensing technologies.

Current research activities span from **molecular biology and biomolecular characterization** to **computational modelling and nanoscale biosensing**, including nanopore-based sensing platforms and graphene field-effect transistor (gFET) biosensors.

The group is currently formed by an Associate Professor, a fixed term researcher, two RTD-A, a post-doc, 3 PhD students and different master students.

Components of the group: Prof. Anna La Teana, Dr. Alice Romagnoli, Dr. Giovanni Di Muccio, Dr. Jesmina Rhexa, Dr. Tiziana Cacciamani, Noemi Borgognoni, Francesco Pignotti

Some Recent Achievements of the PI and the MoLab

Recent research achievements of the PI and the MoLab include contributions to the understanding of biomolecular interactions and the development of nanoscale biosensing technologies, with publications in leading international journals.

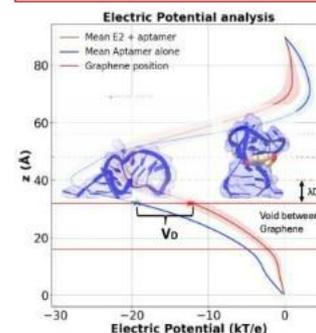
The collage features several scientific publications and journal logos:

- nature communications**: "Lipid-mediated hydrophobic gating in the BK potassium channel" and "Mechanistic snapshots of lipid-linked sugar transfer".
- Cancer Drug Resistance**: "Molecular targeting of the deubiquitinase USP14 to circumvent cisplatin resistance in ovarian carcinoma and identification of novel inhibitors".
- JACS**: "Nanopores with an Engineered Selective Entropic Gate Detect Proteins at Nanomolar Concentration in Complex Biological Sample".
- ADVANCED SENSOR RESEARCH**: "Unlocking the Potential of Field Effect Transistor (FET) Biosensors: A Perspective on Methodological Advances in Computational and Molecular Biology".
- ADVANCED MATERIALS**: "Controlling Electroosmosis in Nanopores Without Altering the Nanopore Sensing Region".
- Biophysical Journal**: "Mapping signal transduction in bistable jumping spider rhodopsin 1".
- PNAS**: "A fixed mutation in the respiratory complex I impairs mitochondrial bioenergetics in the endangered Apennine brown bear".

Logos for **hr** (HR EXCELLENCE IN RESEARCH) and **Open Access** are also visible.



Biomolecular recognition underlies essential biological processes and many diagnostic technologies. Understanding the structural and dynamical mechanisms of biomolecular interactions is therefore key for both fundamental biology and the development of biomedical and biotechnological applications. Advances in molecular simulations, computational biology, and machine learning now enable the study of biomolecular systems at atomic resolution and the rational design of molecules with tailored binding properties. In parallel, nanoscale sensing technologies—such as nanopores and graphene-based field-effect transistors—offer new ways to convert molecular recognition events into measurable electrical signals, opening opportunities for next-generation biosensors and molecular binders.



Research objectives:

- Investigate biomolecular recognition mechanisms (protein–protein, protein–RNA, ligand–receptor) using molecular simulations and computational analysis.
- Develop computational strategies for peptide and molecular binder design targeting interactions of pharmaceutical relevance.
- Study nanoscale biosensing mechanisms in biological nanopores and graphene field-effect transistors (gFETs).
- Support the development of next-generation biosensors, including aptamer-based detection and computational frameworks for signal interpretation.

