

Andrea Pasquadibisceglie, PhD

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I am an Early Career Researcher in the computational structural biology field. I am interested in studying proteins using a computational approach. I got my PhD in Biomedical Sciences and Technologies at the Roma Tre University in 2022, under the supervision of Professor Fabio Polticelli. I am currently a Postdoctoral Fellow employed at the Royal Institute of Technology KTH (Stockholm, Sweden), in the group of Professor Lucie Delemotte, where I am using AI-based algorithms and advanced molecular dynamics methods to study the conformational dynamics of membrane transporters and protein-ligand interactions in ion channels.

EDUCATION

11/2018 –
01/2022

PH.D. IN BIOMEDICAL SCIENCES AND TECHNOLOGIES

Department of Sciences, Roma Tre University, Rome, Italy

- Thesis: “Computational study of the structure and mechanism of mitochondrial carriers involved in human diseases”
- Supervisor: Prof. Fabio Polticelli

10/2015 –
06/2018

MASTER'S DEGREE IN BIOLOGY FOR MOLECULAR, CELLULAR AND PHYSIOPATHOLOGICAL RESEARCH

Department of Sciences, Roma Tre University, Rome, Italy

- Thesis: “Research of spermine oxidase inhibitors for the development of lead compounds”
- Supervisor: Prof. Manuela Cervelli and Prof. Paolo Mariottini

10/2011 –
01/2015

BACHELOR'S DEGREE IN BIOLOGICAL SCIENCE

Department of Biology and Biotechnology “C. Darwin”, Sapienza University of Rome, Rome, Italy

- Thesis: “Neurotrophins role in the Nervous Central System”
- Supervisor: Prof. Mattia Toni

RESEARCH EXPERIENCE

10/2023 –
to date

POSTDOCTORAL FELLOW, KTH ROYAL INSTITUTE OF TECHNOLOGY

Molecular Biophysics Stockholm laboratory, Applied Physics Department of KTH, Science for Life Laboratory, Solna, Sweden
Supervisor: Prof. Lucie Delemotte

- Molecular docking and molecular dynamics simulations of voltage-gated potassium channels and modulators

03/2023 –
09/2023

VISITING RESEARCHER, KTH ROYAL INSTITUTE OF TECHNOLOGY

Molecular Biophysics Stockholm laboratory, Applied Physics Department of KTH, Science for Life Laboratory, Solna, Sweden
Supervisor: Prof. Lucie Delemotte

- Enhanced sampling simulations of mitochondrial carriers based on collective variables derived from AlphaFold2

- 05/2022 – 09/2023** **POSTDOCTORAL FELLOW, ROMA TRE UNIVERSITY**
 Theoretical Biology and Bioinformatics Laboratory, Department of Sciences, Roma Tre University, Rome, Italy
 Supervisor: Prof. Fabio Polticelli
- Modelling and simulations of the conformational dynamics of membrane transporters using AlphaFold2 and molecular dynamics
- 11/2018 – 03/2022** **PH.D. STUDENT, ROMA TRE UNIVERSITY**
 Theoretical Biology and Bioinformatics Laboratory, Department of Sciences, Roma Tre University, Rome, Italy
 Supervisor: Prof. Fabio Polticelli
- Homology modelling and modelling *ab initio* of membrane transporters
 - Molecular dynamics and molecular docking simulations of membrane transporters and ligands
 - Cheminformatics analyses using the RDKit Python library
- 03/2017 – 06/2018** **MASTER'S DEGREE THESIS INTERNSHIP, ROMA TRE UNIVERSITY**
 Molecular Biology Laboratory, Department of Sciences, Roma Tre University, Rome, Italy
 Supervisor: Prof. Manuela Cervelli and Prof. Paolo Mariottini
- Screening of potential spermine oxidase inhibitors, through activity and inhibition assays
 - Molecular docking simulations of spermine oxidase inhibitors
- 09/2016 – 01/2018** **MASTER'S DEGREE INTERNSHIP, ROMA TRE UNIVERSITY**
 Theoretical Biology and Bioinformatics Laboratory, Department of Sciences, Roma Tre University, Rome, Italy
 Supervisor: Prof. Fabio Polticelli
- Protein Homology modelling and modelling *ab initio*
 - Molecular docking
- 05/2015 – 11/2015** **INTERNSHIP, BAMBINO GESÙ CHILDREN'S HOSPITAL**
 Human Microbiome unit, Bambino Gesù Children's Hospital, Rome, Italy
 Supervisor: Dr. Lorenza Putignani
- DNA extraction, fatty acids extraction, PCR

AWARDS

- **Premio Heritage SIB Group Award** (2023, 200 €) – Società Italiana di Biochimica e Biologia Molecolare;
- **C.M. Leric Foundation Scholarship** (16/05/2023-15/09/2023, 50 000 SEK) to carry out the project "Investigation of mitochondrial carriers transport mechanism combining artificial intelligence and molecular dynamics techniques" in Prof. Lucie Delemotte's laboratory (SciLifeLab, KTH Royal Institute of Technology - Stockholm, Sweden);
- **FEBS Short-Term Fellowship** (15/03/2023-15/05/2023, 5 790 €) to carry out the project "Characterization of the conformational dynamics of the mitochondrial carrier family" in Prof. Lucie Delemotte's laboratory (SciLifeLab, KTH Royal Institute of Technology - Stockholm, Sweden).