

Zoé GRIMANELLI

Computational and Structural Biology | Molecular Modeling | Drug Discovery

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PhD in cell and computational biology, with strong expertise in structural biology, molecular modeling and analysis of pharmacologically and clinically relevant data. Experienced in interdisciplinary research bridging molecular simulations, drug mechanisms and disease biology, with an interest in pharmaceutical R&D.

EDUCATION AND QUALIFICATIONS



Master's course at POLYTECH NICE SOPHIA – Bioinformatics major

Master of Science

Drug design, modeling of biological networks, structural biology, biostatistics
Algorithmics, Machine Learning

2019-2022

*Sophia-Antipolis,
France*



Preparatory class at SORBONNE UNIVERSITE – Biology major

Ranked 4th in the final national competitive exam

Cellular and molecular biology, pharmacology, biotechnology, biochemistry
Chemistry, physics, statistics
Management, regulatory affairs

2017-2019

Paris, France

PROFESSIONAL EXPERIENCE



Institut de Pharmacologie Moléculaire et Cellulaire – IPMC-CNRS
Côte d'Azur University

Ph.D. student, team « dynamics of lipid membranes »

Team leader: Dr. Bruno Antonny

Supervisors: Dr. Bruno Mesmin and Dr. Romain Gautier

(mesmin@ipmc.cnrs.fr, gautier@ipmc.cnrs.fr)

2022 – 2025

Sophia-Antipolis, France

Thesis: "OSBP and the VAP twins in motion: dynamics, partners, and structural organization at membrane contact sites"



Bayer AG

Computational Molecular Design intern

Team leader: Dr. Clara Christ, Supervisor: Dr. Lukas Braun

Drug Design – Modeling and simulations of protein complexes

Writing scripts in Python and Bash

February-July 2022

Berlin, Germany



Università Roma Tre

Computational biology intern

Team Leader: Pr. Fabio Polticelli

Structural study of a mitochondrial transporter with molecular dynamics simulations

June-August 2021

Rome, Italy

SKILLS

Sciences:

Programming (Python), statistical analysis of biological data (R), computational modeling and simulations, drug design, molecular and cellular biology, pharmacology, biochemistry

Languages:

French, German: Native (French-German Baccalaureate), **English:** Bilingual (TOEIC: 990/990)

Communication:

Scientific presentations (posters, conferences, public speaking competition),
scientific writing (research articles, grant applications)

Transversal:

Coordination of cross-functional scientific projects (clinical, experimental and modeling),
experimental planning and deliverables tracking
teaching and student supervision

RESEARCH EXPERIENCE – Ph.D.

Research topic:

Structural and functional analysis of membrane protein complexes involved in cholesterol transport through integrated cell biology and molecular modeling approaches, contributing to the understanding of drug action, biological system dynamics and disease mechanisms, in collaboration with clinicians.

Publications:

- Grimanelli Z. *et al.* N-terminal truncation of VAPA leads to disturbed membrane contact sites between endoplasmic reticulum and pulmonary lamellar bodies, and severe syndromic disease in humans (under review)
Identification of a novel cholesterol transport mechanism in pulmonary lamellar bodies, based on the study of the first VAPA protein mutant identified in a patient with severe pulmonary fibrosis.
- Grimanelli Z., Mesmin B., Gautier R. Docking and Molecular Dynamics Simulations of ORPphilins Targeting OSBP. Methods in Enzymology. 2025 Dec 23. doi: 10.1016/bs.mie.2025.11.021.
Methodology article on the study of ligand–receptor interactions using docking and molecular dynamics simulations, based on the strategy presented in (Jézéquel G., Grimanelli Z. et al., 2024)
- Jézéquel G., Grimanelli Z. *et al.* Minimalist Natural ORPphilin Macarangin B Delineates OSBP Biological Function. J Med Chem. 2024 Dec 20. doi: 10.1021/acs.jmedchem.4c01705.
Study describing a new inhibitor of the OSBP protein, which reduces Zika virus replication and suggests potential for the development of antiviral therapies.
- Subra M., Grimanelli Z., Gautier R., Mesmin B. Stranger Twins: A Tale of Resemblance and Contrast Between VAP Proteins. Contact (Thousand Oaks). 2023 Jul 12. doi: 10.1177/25152564231183897.
Review exploring the similarities and differences between the VAPA and VAPB proteins.

Conferences:

- Poster: Group of Graphism and Molecular Modeling (GGMM) (Normandy, France) – June 2025
Toward a coarse-grained model of a Membrane Contact Site: steps and challenges
Grimanelli Zoé, Gautier Romain, Mesmin Bruno
- Poster: EMBO Workshop “The ER: Guardian of Cellular Homeostasis” (Barga, Italy) – October 2024
VAPA vs VAPB: exploring divergences in structure, dynamics and function
Grimanelli Zoé, Pradelli Clara, Subra Mélody, Antonny Bruno, Gautier Romain, Mesmin Bruno

Additional Activities:

- Supervision of a final-year bioinformatics project for a group of students at Polytech
- Participant in the 2025 international competition “Three Minute Thesis” – science communication for the general public.

[Link to the video](#)



OTHER ACTIVITIES

Volunteering:

Puritas-Hayleys Group, (Colombo, Sri Lanka) – April-June 2017
Installing water treatment plants in rural areas
Donation management for 2017 flood victims

Interests:

Figure skating (4 years of practice), ballet (8 years at the conservatory)
Scientific readings, novels