



DAVIDE PIETRAFESA

Bioinformatician | PhD student



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<http://github.com/cidoimo>
<https://linktr.ee/biodhave>

Research Experience

● Ph.D. student

University of Rome "Tor Vergata" | Lab. of Structural Bioinformatics | Apr 2023 - present

Main project

Molecular modeling of the HuR protein. Design, docking and simulation of RNA aptamers in order to develop potential cancer therapies.

Side projects

Deciphering the role of trehalose in the *Chroococcidiopsis* 029 high desiccation tolerance. Experimental determination and simulative analysis of the 30S ribosomal subunit.

Phylogenetic analysis and *in silico* characterization of hemoglobins structure of iguanas: a multi-oriented approach.

In vitro and *in silico* characterization of Palmitic acid with a potential antitumor activity targeting human DNA Topoisomerase IB.

In silico evaluations of the possible molecular interaction between ultrafine airborne particulate matter (PM1.0) and SARS-CoV-2

Expertise

Homology modeling ● Ab-initio modeling ● Aptamers design ● Virtual screening ● Molecular docking ● Bash scripting ● Python scripting ● R scripting ● Genomic alignment ● AMBER2022 ● Gromacs 2022 ● NAMD ● Molecular Dynamics ● High Parallel Computing (HPC) ● Gaussian accelerated Molecular Dynamics (GaMD) ● VMD ● Pymol ● UCSF CHIMERA

● Undergraduate student internship

Italian Agency for New Technologies, Energy and Sustainable Economic Development (ENEA) | Lab. of Structural Bioinformatics | Oct 2021 - Jul 2022

Main project

Molecular Modeling and Molecular Dynamics simulations of acid β -Glucosidase dimers to understand the effect of a Parkinson-associated mutation.

Expertise

Bash scripting ● Python scripting ● Haddock ● HEX ● Molecular Docking ● CHARMM-GUI ● VMD ● Gromacs 2019 ● Molecular Dynamics ● High Parallel Computing (HPC)

Education

● Ph.D. in Materials for Health, Environment and Energy

University of Rome "Tor Vergata" | Apr 2023 - present

Ph.D. project

"Computational design of RNA aptamers targeting the HuR protein as a promising therapeutic strategy for cancer"

Supervisor Prof. Mattia Falconi

Co-supervisors Prof. Manuela Helmer-Citterich | Federico Iacovelli, Ph.D.

● M.Sc. Bioinformatics

University of Rome "Tor Vergata" | Sept 2020 - Jul 2022 | 110 summa cum laude

Thesis

"Effect of a Parkinson's-associated mutation (E326K) on the structure, stability and dimerization of acid β -Glucosidase protein: a high-performance classical molecular dynamics study"

Supervisor Caterina Arcangeli, Ph.D.

Co-supervisor Prof. Mattia Falconi

● B.Sc. Biological Sciences

University of Salerno | Sept 2017 - Sept 2020 | 110 summa cum laude

Thesis

"The role of Tetrabenazine and its derivatives in Parkinson's disease treatment"

Supervisor Prof. Margherita De Rosa

Digital skills

Homology modeling ● *Ab-initio* modeling ● AlphaFold ● D-I Tasser ● Virtual screening ● Molecular Docking simulations ● AutoDock VINA ● Bash ● Python ● R ● AMBER suite ● Gromacs suite ● NAMD suite ● Molecular Dynamics simulations ● High Parallel Computing (HPC) ● VMD ● Pymol ● UCSF CHIMERA ● RNAfold ● MC-fold ● MC-sym ● ROSETTA ● Social Media Management

Scientific interests

Cancer research ● Molecular modeling ● Molecular Dynamics ● Molecular Docking ● Chemo-informatics ● Structural Biology ● Structural Bioinformatics ● Computational Biology ● Computational Genomics

Additional academic contribution

● Supervision of master thesis students

● Freelance Social Media Manager for M.Sc. Degree in Bioinformatics

University of Rome "Tor Vergata" | Jul 2023 - present

Management of academic contents, updates, and news on the MSc Degree in Bioinformatics website (<https://lmbioinfo.bio.uniroma2.it>), Facebook and Instagram (@lmbioinfo_torvergata)

Publications

- Structural and functional effects of the Parkinson-associated E326K mutation: an *in silico* approach

D Pietrafesa, A Casamassa, M Santoro, M Marano, C Consales, JD Rosati, C Arcangeli

In progress

Certifications

- Spring 2021 Virtual Applied Data Science Training Institute Program (VADSTI)
Howard University | Oct 2021
- Google IT Certificate
Google & Academy Rapido | Dec 2021
- Online Summer School on Parallel Computing
CINECA | Jul 2022
- High-performance Bioinformatics
CINECA | Dec 2022

Languages

- Italian (first language)
- English (C1)
- Spanish (A1)

"I authorize the processing of my personal data in the CV, pursuant to Legislative Decree June 30, 2003, no. 196 'Code regarding the protection of personal data' and GDPR (EU Regulation 2016/679)."

Rome, 02/01/2024

