

Vito Genna, Ph.D.

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Senior Research Scientist

Principal Investigator

Computational Chemistry/Biochemistry

Molecular Modeling, Structural Genomics, and Synthetic Biology

Profile Summary

Senior/Principal Computational Chemist with a Ph.D. in Biochemical Sciences and Biotechnologies and extensive research experience in academic and industrial environments. Highly regarded in the field of theoretical chemistry with specialization in DNA/RNA/enzyme characterization and engineering, gene silencing, multiscale molecular dynamics simulations including hybrid quantum chemistry, free energy calculations, and high-performance computing (HPC). Designs and leads national and international research projects focused on deciphering enzymatic reaction mechanisms and engineering nucleic acids for therapeutic purposes using a range of HPC chemistry technologies and tools. Enjoys working with and lead diverse, multi-disciplinary, multicultural teams to brainstorm new methods for solving complex scientific challenges. Sharp technical acumen with proficiency in various systems, software applications, and programming languages (Python, bash). Numerous presentations at international conferences and publications in high-quality international scientific journals. Adaptable and fast-learning with strong data analysis, critical thinking, and complex problem solving skills.

Areas of Expertise

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|------------------------------------|-----------------------------------|------------------------------------|
| ◆ Scientific Research and Studies | ◆ Computational (Bio)Chemistry | ◆ Biophysics and Bioinformatics |
| ◆ High-Performance Computing (HPC) | ◆ Cancer | ◆ Free Energy Approaches |
| ◆ Quantum Mechanics (QM/MM) | ◆ Nucleic Acids and Enzymology | ◆ DNA/RNA/Enzyme Engineering |
| ◆ Machine Learning (ML) | ◆ Artificial Intelligence (AI) | ◆ Molecular Dynamics Simulations |
| ◆ Drug Discovery and Development | ◆ Free Energy Calculations | ◆ Grant Writing and Fund Raising |
| ◆ Project Design and Management | ◆ Laboratory Management | ◆ Lab Technologies and Instruments |
| ◆ Database Design and Management | ◆ Research Methods and Techniques | ◆ Data Analysis and Integration |

Education

Doctor of Philosophy in Biochemical Sciences and Biotechnologies, April 2017

University of Bologna, Bologna, Italy/Italian Institute of Technology, Genova Italy

Dissertation: "Multiscale Simulations to Dissect Enzymatic Processing of Nucleic Acids"

Master of Science in Biochemistry, February 2013

University of Cagliari, Cagliari, Cagliari, Italy

Thesis: "Bioinformatics Investigations to Select Promising Inhibitors for HIV-2 Reverse Transcriptase"

Bachelor of Science in Molecular Biology, *cum laude*, June 2011

University of Cagliari, Cagliari, Cagliari, Italy

Thesis: "Structural Comparison between Reverse Transcriptases of HIV-I and HIV-II Viruses"

Research Experience

Senior Consultant

January 2020 – Present

- Provide professional consulting to biotechnical and pharmaceutical companies to help overcome biochemical and technology advancement challenges in the area of HPC.
- Assisted multiple small- to medium-sized biotechnology companies such as *CompChem Solutions*, *Nostrum Biodiscovery*, *BiCycle* and *KolabTree*.
- Addressed their scientific needs and suggested effective strategies for technically overcoming scientific challenges with molecules to achieve promising therapeutic advancements or biotech applications.

Vito Genna, Ph.D.

Spanish Ministry of Health, Barcelona, Spain
Senior Scientist | Project Manager at IRB Barcelona

February 2020 – Present

- Led the team in developing and implementing high-impact research strategies and plans and coordinating scientific exchanges to analyze the host-selection mechanism of SARS-CoV-2.
- Characterized and discovered the evolutionary path of SARS-CoV-2 virus.
- Created mutation tracking system and database to assist in localizing crucial mutations for vaccine development.
- The research results will help to anticipate the next evolutionary step of other viruses to avoid a future pandemic.
- Supervised and mentored Ph.D. students.

European Molecular Biology Organization (EMBO), Barcelona, Spain
Senior Scientist | Project Manager, Excellence in Life Sciences Project

June 2018 – February 2020

- Awarded an esteemed grant to engineer pharmaceutically-relevant nucleic acids to counteract and prevent the spread of cancer with an experimentalist team in Cambridge, U.K.
- Selected from an applicant pool of 3,000+ scientists across Europe.
- Successfully engineered a nucleic acid with potent anticancer activity.
- Applied various scientific methods including bioinformatics, QM/MM molecular mechanics, and force-field-based molecular dynamics simulations.
- Published more than 20 scientific articles and book chapters in several top-tier peer-reviewed scientific journals.
- The DNA modification may be patented in the next two years as a new class of anticancer molecules.
- Supervised and mentored Ph.D. students.

Italian Institute of Technology, Genova, Italy
Scientist

September 2015 – January 2018

- Collaborated with a multicultural team in the transversal drug discovery department focused on fighting melanoma skin cancer by dissecting Polymerase- η functioning by means of extensive high-performance scientific computing.
- Set up and performed theoretical calculations on high-performance computing machines and submitted weekly reports.
- Employed different scientific methods including bioinformatics, QM/MM, and molecular dynamics simulations.
- Supervised and mentored Ph.D. students.

Forschungszentrum Jülich, Jülich, Germany
Internship, Scientist (Marco Polo Fellowship)

August 2014 – August 2015

- Investigated the reaction mechanism of DNA Polymerase- η to better understand the biological basis of melanoma onset in humans.
- Gained in-depth knowledge in hybrid QM/MM approaches working with Professor Carloni, one of the most renowned scientists in the field.
- Supervised and mentored master-level students.

Vito Genna, Ph.D.

École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland
Junior Scientist | Department of Bioengineering

February 2013 – September 2013

- Studied the mathematical concept of Newtonian molecular dynamics simulations, a fundamental technique of theoretical chemistry.
- Collaborated with a project team to successfully characterize magnesium metal ion and human enzymes.
- Co-authored and published several manuscripts on the topic in top-tier international peer-reviewed journals.

Centro Nacional de Investigación Oncológicas, Madrid, Spain
Internship, Junior Scientist (Erasmus Placement Fellowship)

March 2009 – August 2009

Development & Training

Leadership Programme, European Molecular Biology Organization, Heidelberg, Germany, 2020

Effective Science Communication, European Molecular Biology Organization, Heidelberg, Germany, 2019

PLUMED: Boost your Free energy calculations, Belfast, Ireland, 2016

Understanding Molecular Dynamics Simulations, Amsterdam, Holland, 2015

Honors & Awards

Doctor Mundi, University of Bologna, April 2017

Marco Polo Fellowship, University of Bologna, August 2014 – August 2015

Best Student of the Year and special recognition for completion of the Master Degree in 14 months, University of Cagliari, 2013

Erasmus Placement Fellowship, University of Cagliari, March 2009 – August 2009

Publications

Full publication details available on Google Scholar <https://scholar.google.com/citations?user=IJh0ProAAAAJ&hl=it>

Grants & Funding

Raised ~\$500K and more than \$200K in computational grants and resources awarded via proposal submission and panel evaluation, including funding from the John Von Newman Computational Center

Technical Proficiencies

Systems: LSF, Unix/Linux distro for High-Performance Computing, MacOS, SLURM, PBS

Software: Gromacs, Amber, Terachem, Gaussian, PyMol, VMD, Orca, NAMD, PLUMED, Chimera, SQL, Microsoft Office (Excel, Word), Gnuplot, Grace.

Programming Languages: Python, Bash Scripting.