Lara CALLEA, *PhD* Curriculum Vitae

NATIONALITY: Italian

DATE OF BIRTH: 13/10/1992

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ORCID: https://orcid.org/0000-0003-0071-601X

EDUCATION AND TRAINING

01/2024-present **Post-doctoral research**
University of Milano-Bicocca, Milano (MI) Italy

▪ Project in Computational Chemistry (SSD CHIM/03):
"*Computational study of the molecular determinants of oxygen resistance in [FeFe] hydrogenases*"
Supervisors: Prof. Claudio Greco, Prof. Luca Bertini

04/2022-12/2023 **Post-doctoral research**
University of Milano-Bicocca, Milano (MI) Italy

▪ Project in Computational Chemistry (SSD CHIM/02):
"*Computational studies of ligand-protein binding using molecular dynamics approaches*"
Supervisor: Prof. Laura Bonati

11/2018-05/2022 **PhD course in Chemical, Geological and Environmental Sciences**
Curriculum Chemical Sciences
University of Milano-Bicocca, Milano (MI) Italy

▪ Project in Computational Chemistry (SSD CHIM/02):
"*Modeling of ligand-protein binding with advanced molecular dynamics methods*"
Supervisor: Prof. Laura Bonati

03/2021-08/2021 **Blended mobility period**
Institute for Advanced Simulation (IAS), Forschungszentrum Jülich
under the supervision of the Prof. Paolo Carloni

05/2018-10/2018 **Research fellowship**
University of Milano-Bicocca, Milano (MI) Italy

▪ Project in Computational Chemistry:
"*Role of dynamics in the modelling of the interaction between ligands and PX receptor*"

10/2015-03/2018 **Master's Degree in Chemical Sciences and Technology, 109/110**

University of Milano-Bicocca, Milano (MI) Italy

- Master's Degree Project in Computational Chemistry:
  "*Dynamics in ligand-protein interactions: modelling of binding to PXR*"

10/2011-11/2015 **Bachelor's Degree in Chemical Sciences and Technology, 93/110**

University of Milano-Bicocca, Milano (MI) Italy

- Bachelor's Degree Project in Computational Chemistry:
  "*Computational study of inhibitors to HIF-2α protein*"

09/2006-07/2011 **Scientific High School Diploma, 100/100**

Higher Education Institute Euclide, Contrada Monoscalco, Bova Marina (RC) Italy

TEACHING EXPERIENCES

10/2025-10/2025 **Adjunct Professor**
University of Milano-Bicocca, Milano (MI)
Laboratory of General Chemistry within the Bachelor's Degree Program in Biological Sciences.

05/2023-06/2023 **Laboratory assistant**
University of Milano-Bicocca, Milano (MI)
Laboratory of Physical Chemistry II within the Chemical Sciences and Technology Bachelor's Degree.

05/2019-06/2019 **Laboratory assistant**
University of Milano-Bicocca, Milano (MI)
Laboratory of Physical Chemistry II within the Chemical Sciences and Technology Bachelor's Degree.

PERSONAL SKILLS

Mother tongue(s) Italian

English B2

Communication skills
- Good communication skills gained thanks to team working and oral presentations during PhD course

Organisational / managerial skills
- Problem-solving
- Analytical
- Interpersonal
- Team member

Digital competence
- Good knowledge of Linux operating systems
- Basic Bash and Python programming skills
- Basic knowledge of R environment for statistical analysis

- Advanced experience in use of software for molecular modelling and simulations (Gromacs, Plumed, Schrödinger Suite, BiKi Life Sciences tools)
- Advanced experience in use of software for molecular graphics (Schrodinger Suite, Pymol, VMD)
- Advanced knowledge of office suite - European Computer Driving Licence (word processor, spread sheet, presentation software)

ADDITIONAL INFORMATION

Publications

- Motta, S., **Callea, L.**, Mulla, S. I., Davoudkhani, H., Bonati, L. & Pandini, A. SOMMD: an R package for the analysis of molecular dynamics simulations using self-organizing map. Bioinformatics 41, btaf308 (2025).
- **Callea, L.**, Caprai, C., Bonati, L., Giorgino, T. & Motta, S. Self-organizing maps of unbiased ligand–target binding pathways and kinetics. J. Chem. Phys. 161, 135102 (2024).
- Bonati, L., Motta, S. & **Callea, L.** The AhR Signaling Mechanism: A Structural Point of View. J. Mol. Biol. 436, 168296 (2024).
- Raghavan, B., Paulikat, M., Ahmad, K., **Callea, L.**, Rizzi, A., Ippoliti, E., Mandelli, D., Bonati, L., De Vivo, M. & Carloni, P. Drug Design in the Exascale Era: A Perspective from Massively Parallel QM/MM Simulations. J. Chem. Inf. Model. 63, 3647–3658 (2023).
- Basciu, A., **Callea, L.**, Motta, S., Bonvin, A. M. J. J., Bonati, L. & Vargiu, A. V. in Annu. Rep. Med. Chem. (ed. Caballero, J.) 43–97 (2022).
- Motta, S., **Callea, L.**, Bonati, L., Pandini, A., *PathDetect-SOM: A Neural Network Approach for the Identification of Pathways in Ligand Binding Simulations.* J. Chem. Theory Comput. (2022).
- **Callea, L.**, Bonati, L., Motta, S., Metadynamics-Based Approaches for Modeling the Hypoxia-Inducible Factor 2α Ligand Binding Process. J. Chem. Theory Comput. 17, 3841–3851 (2021).
- Motta, S., **Callea, L.**, Tagliabue, S. G. & Bonati, L. Exploring the PXR ligand binding mechanism with advanced Molecular Dynamics methods. *Sci. Rep.* 8, 16207 (2018).

Conferences

- BBCC2021, Bioinformatics and Computational Biology Conference, Online (01/12/2021-03/12/2021)
- SCI2021, XXVII Congresso Nazionale della Società Chimica Italiana, Online (14/09/2021 - 23/09/2021)
- *Women in the sciences*, University of Milano-Bicocca, Milano, Italy (14/05/2019)
- *Open Day 3Rs: Refinement, Reduction, Replacement*, University of Milano-Bicocca, Milano, Italy (31/10/2018)
- 5th CDDD Meeting - *Computationally Driven Drug Discovery*, IFOM, Milano, Italy (16/11/2017 - 17/11/2017)
- Horizon Chem 2016 - *La chimica moderna in Horizon 2020: la risorsa acqua, sfide ed opportunità per l'Europa*, University of Milano-Bicocca, Milano, Italy (09/03/2016)
- Horizon Chem 2015 - *Le sfide di Horizon 2020 per la chimica moderna: salute ed energia, affrontare i sistemi complessi con modelli computazionali*, University of Milano-Bicocca, Milano, Italy (06/03/2015)
- Horizon Chem 2014 - *Verso le eccellenze scientifiche di Horizon 2020: nuove sfide per la chimica*, University of Milano-Bicocca, Milano, Italy (24/01/2014)

Conference presentations

- Motta S., **Callea L.**, Bonati L., Pandini A. *A Neural Network Approach for the Identification of Pathways in Molecular Dynamics Simulations of Ligand Binding*, BBCC2021: Bioinformatics and Computational Biology Conference (**oral**)
- Motta S., **Callea L.**, Bonati L. *Study of ligand binding to HIF-2α through Path-Metadynamics,* SCI2021: XXVII Congresso Nazionale della Società Chimica Italiana (**oral**)
- **Callea L.**, Motta S., Bonati L. *Modeling of ligand binding to the HIF-2α protein with enhanced sampling methods*, CECAM School "BImBS 2019 - BioInformatics meets BioSimulations in protein and DNA studies: from theory to practice" (**poster**)
- **Callea L.**, Motta S., Giani Tagliabue S., Bonati L. *Role of Dynamics in ligand-protein interactions: modelling of binding to Pregnane X Receptor*, BioExcel Summer School on Biomolecular Simulations 2018, Pula, Italy 2018 (**poster and oral**)

Schools

- CECAM School “Hybrid Quantum Mechanics / Molecular Mechanics (QM/MM) approaches to biochemistry and beyond”, CECAM-HQ-EPFL, Lausanne, Switzerland (16/05/2022 – 20/05/2022)
- CECAM School "BImBS 2019 - BioInformatics meets BioSimulations in protein and DNA studies: from theory to practice", USI, Lugano, Switzerland (5/10/2019 – 12/10/2019)
- Data Carpentry Workshop, University of Milano-Bicocca, Milano, Italy (14 - 15/02/2019)
- BioExcel Summer School on Biomolecular Simulations 2018, Science and Technology Park of Sardinia, Pula, Italy (18/06/2018 - 22/06/2018)