

PERSONAL DETAILS

Family name, first name: Cavalli, Andrea

Researcher unique identifier (ORCID): 0000-0002-6370-1176

URL: <https://www.cecarn.org/>

EDUCATION AND KEY QUALIFICATIONS

1996-1999 PhD, Pharmaceutical Sciences, University of Bologna, Italy (graduated 21/12/1999)

1990-1996 Bachelor's and Master's Degree, Pharmaceutical Chemistry and Technology, University of Bologna, Italy

CURRENT POSITIONS

2023-present Director, Centre Européen de Calcul Atomique et Moléculaire (CECAM) & Professeur Titulaire, École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland

2023-present Collaborator, Italian Institute of Technology (IIT); Co-founder, Center for Clinical and Computational Genomics (C3G), Aosta, Italy

2014-present Professor of Medicinal Chemistry, University of Bologna, Italy (on leave for directorship)

PREVIOUS POSITIONS

2021-2022 Vice-Scientific Director, Istituto Italiano di Tecnologia (IIT), Genova, Italy

2017-2022 Associate Director for Computational Sciences; Department Director, Computational & Chemical Biology, IIT, Genova, Italy

2018-2022 Coordinator, PhD Program in Data Science & Computation (University of Bologna, IIT, INFN)

2019-2024 Co-Director, CMP³VdA (overall budget from an external grant: 10+ M€); now, C3G-Center for Clinical and Computational Genomics, Aosta, Italy

2019 Visiting Scientist at the SKAGGS School of Pharmacy and Pharmaceutical Sciences of the University of California, San Diego, USA

2017-2022 Chair, QSAR, Chemoinformatics & Modeling Society (www.qsar.org)

2001-2014 Assistant and Associate Professor in Medicinal Chemistry, University of Bologna, Italy

2008-2013 Senior Researcher in Computational Chemistry, IIT, Genova, Italy

1999-2001 Postdoctoral Fellow in Computational Biophysics, SISSA, Trieste, Italy

2001, 2002 Visiting Scientist at the Department of Chemistry and Applied Biosciences of ETH, Zurich, Switzerland

RESEARCH ACHIEVEMENTS AND PEER RECOGNITION

Prof. Cavalli developed and applied computational methods, bioinformatics pipelines, and AI tools for drug discovery and precision medicine. Porting to high-performance computing (HPC) and hybrid CPU-GPU infrastructures has been a further keystone of his scientific/technological activities. He published more than **350 papers** (h-index 82, citations ~25,000) and delivered over **150 invited lectures** and seminars at international congresses and research institutions. He is an inventor in **12 international patents**.

https://scholar.google.it/citations?hl=it&user=4xTOvaMAAAAJ&view_op=list_works

Awards and distinctions

2026 Invited seminar tour: Academia Sinica (Taipei), RIKEN, Tsukuba University, and Kyoto University (Japan). Five seminars on physics-based modeling in computational drug discovery, and AI-driven methods and bioinformatics for precision medicine

2024 Nomination for Associate Membership, Sigma Xi, The Scientific Research Honor Society

2017 Angewandte Chemie Int. Ed., Outstanding Reviewer – Top 5%

2017 Journal of Medicinal Chemistry, Outstanding Reviewer

2010 Paper *J. Am. Chem. Soc.* 2010, 132, 7361 highlighted by Prof. Jorgensen (Yale) in *Nature* 2010, 466, 42

2003 Farmindustria Prize for Pharmaceutical Research (dedicated to scientists under 40)

1996 Rotary Prize, Best Student of the Year, Faculty of Pharmacy, University of Bologna

Selected invited plenary/keynote lectures (from >150)

July 2026 Role of AI and high-performance computing in precision medicine, Invited seminar to celebrate the 50th birthday of the Department of Chemistry of the University of Aveiro, **Aveiro, Portugal**

Apr. 2026 Genomics meets AI towards applications in precision medicine, RIKEN Center for Integrative Medical Science, **Yokohama, Japan**

Apr. 2026 Dynamical docking and binding free energy via enhanced sampling methods, Tsukuba University, **Tsukuba, Japan**

Jan. 2026 Fully dynamical docking via molecular dynamics and related methods, two invited webinars, **Pfizer Global (27/1/26) & Microsoft Global (28/1/26)**

Sep. 2025 Molecular dynamics and related methods in drug discovery, Quantum Chemistry for Drug Design: From Theory to Applications, **Prague, Czech Republic**

July 2025 Towards fully dynamical docking via MD and related methods, QUITEL2025 – 48th Congress of Theoretical Chemists of Latin Expression, **Cartagena, Colombia**

July 2024 Role of molecular dynamics and related methods in drug discovery, Frontiers of Computational Reaction Prediction, CECAM Flagship Workshop, **University of Chicago, USA**

May 2024 Physics-based approaches to computational drug discovery, International Society of Quantum Biology and Pharmacology President's Meeting, **Athens, Greece**

Feb. 2024 Role of molecular dynamics and related methods in drug discovery, MD@60 (to celebrate 60 years after the pioneering paper by A. Rahman, Phys. Rev. 136, A405-A411 (1964)), JNCASR, **Bangalore, India**

Nov. 2023 Physics-based approaches to computational drug discovery, QUITEL2023 – 46th Congress of Theoretical Chemists of Latin Expression, **Montevideo, Uruguay**

Apr. 2023 The neurokinome in drug discovery: triple protein kinase inhibitors, a possible path forward, ACS Spring 2023, **Indianapolis, USA**

ADDITIONAL INFORMATION

Prof. Cavalli has served on the editorial boards of several international journals and has acted as a referee for *Nat. Chem.*, *Nat. Commun.*, *PNAS*, *Angew. Chem. Int. Ed.*, *J. Am. Chem. Soc.*, *J. Med. Chem.*, and others. I have reviewed grants for the European Commission (including ERC), HFSP, the Austrian Science Fund, the Swiss National Science Foundation, the Israel Science Foundation, the Alzheimer's Association (USA), ANR (France), NCBiR (Poland), the Research Council of Norway, and ANVUR (Italy).