

2021 Hans & Marlies Zimmer International Scholar

Paolo Carloni

Director of the Institute “Computational Biomedicine” (IAS-5/INM-9)

Forschungszentrum Jülich GmbH, Jülich, Germany

Professor of Theoretical Biophysics, Physics Department,

RWTH Aachen University, Aachen, Germany



(Picture by FZJ Sascha Kreklau)

- Current Position: Professor for Theoretical Biophysics and Institute Director in Jülich
- Education/Training:

1990: Diploma (Chemistry), University of Florence, Italy

1994: Ph.D. (Chemistry, majoring Computational Biophysics), University of Florence, Italy
(Supervisors: Michele Parrinello, Lucia Banci, PierLuigi Orioli)

- Positions and Scientific Appointments:

2018 – present: Co-Director of the JARA Center for Simulation and Data Science (JARA CSD), Research Center Jülich and RWTH Aachen University

2016 – present: Director of the JARA-Institute for Molecular Neuroscience and Neuroimaging (INM-11), Research Center Jülich and RWTH Aachen University

2016 – present: Co-Director of Key Science Laboratory on Multiscale Simulations of Complex Systems, University of Hanoi, Vietnam

2013 – present: Director of the Institute for Computational Biomedicine (INM-9), Institute for Neuroscience and Medicine, Research Center Jülich

2012 – present: Director of the Institute for Computational Biomedicine (IAS-5), Institute for Advanced Simulation, Research Center Jülich

2009 – present: Full Professor (W3) for Theoretical and Computational Biophysics, RWTH Aachen University
2009 – 2014: Professor at the German Research School (GRS), Jülich
2004 – 2009: Full Professor in Chemistry, International School for Advanced Studies (SISSA), Trieste
2000 – 2004: Associate Professor in Chemistry, International School for Advanced Studies (SISSA), Trieste
1998 – 2000: Assistant Professor in Chemistry, International School for Advanced Studies (SISSA), Trieste
1995 – 1997: On leave at University of Florence, Researcher at IBM Research Laboratory, Zurich
1994: Assistant Professor in Chemistry, University of Florence
1993 – 1994: Postdoc, Dept. Chemistry, University of Florence
1990 – 1992: Visiting scientist, IBM Zuerich Research Laboratory (Dr. Michele Parrinello), & IBM Kingston (Prof. E. Clementi), New York

- Contributions to Science:

Paolo Carloni has developed and used multiscale methods in molecular simulation (from quantum to coarse grain) aimed at understanding structure/function of biomolecules and their complexes. He has contributed to the modeling of metal ions in biological systems, to the understanding of reaction mechanism of enzymatic superfamilies (such as that of the proteases), to molecular mechanisms of drug resistance, to the investigation of RNA/drug binding, and, more recently to providing insight on the function and the signaling cascades of neuroreceptors. Many of his papers are in collaboration with experimental groups. He has devoted a major effort to high level education (as for today, he has supervised more than 50 PhD students).

- Google scholar: https://scholar.google.com/citations?user=G2R_F1sAAAAJ&hl=en

Title and Abstract:

Multiscale simulations of neuronal G-protein coupled receptors

G-protein coupled receptors (GPCRs) play a paramount role for diverse brain functions, from chemical sensing and synaptic transmission to behavior. Here we will describe our current efforts in developing and applying multi scale molecular simulation studies (from quantum to coarse grain) to shed light on neurobiologically relevant processes involving GPCRs. This knowledge may be used to identify new ligands interfering with neurological diseases.