Paolo Calligari —— Curriculum Vitae

Present Affiliation

Dept. of Chemical Sciences and Technologies
University of Rome - Tor Vergata
Via della Ricerca Scientifica
I-00133, Rome
Italy

email: paolo.calligari@uniroma2.it
email: paolo.calligari@gmail.com
url: http://sites.google.com/site/paolocalligari/
ORCID: 0000-0001-7614-8931

Professional Experiences

2021-present Researcher
Department of Chemical Science and Technology - Università degli Studi di Roma - "Tor Vergata" (Italy)

2017-2020 Post-doctoral researcher
Department of Chemical Science and Technology - Università degli Studi di Roma - "Tor Vergata" (Italy)

2014-2017 Post-doctoral researcher
Department of Chemistry - Università degli Studi di Padova (Italy)
Theoretical Chemistry Group

2012-2014 Post-doctoral researcher
International School for Advanced Studies - SISSA - Trieste (Italy)
NOFYSAS 2012 - Research grants for young researchers

2009-2012 Post-doctoral fellow,
Ecole Normale Supérieure, Paris (France)
2009-2010 European Grant: I3 - Integrated Infrastructure Initiative.
2010-2011 ENS post-doctoral fellowship
2011-2012 ANR "Conception et Simulation" Project: SPUTNIK - Simulating experiments for the study of protein structure and dynamics.

Education

2004-2008 **Ph.D.** (Mention: Très honorable) - highest distinction
Université Pierre et Marie Curie, Paris, France
Ecole Doctorale Interface de la biologie avec la chimie, la physique et l'informatique
Thesis supervisor: Prof. Gerald R. Kneller, CNRS Orléans
Co-supervisor: Prof. Mark Johnson, Institut Laue Langevin, Grenoble
Thesis text: *Signature of protein adaptation to "warm deep sea" environment : the case of the Initiation Factor 6 studied by molecular dynamics and neutron scattering*.
Date of defence: 18 December 2008.
Equipollenza con "Dottorato di Ricerca": Decreto Ministeriale n. 163 del 18/03/2015
short keyword : **PhD**

2001-2002 ERASMUS - Student exchange program (10 months)
Ecole Normale Supérieure, Lyon, France
Lectures: Biochemistry, Molecular Biology, Statistical Physics

1999-2004

Laurea in Fisica, Indirizzo Fisica dei Biosistemi
Università degli Studi *La Sapienza*, Rome, Italy
Supervisor: Dr. Andrea Giansanti
Thesis: *Sequenze, matrici binarie e folding proteico*.

Awards and Funding

2020 **Qualified for applying to positions in Italian Universities as Assistant Professor.**
Fields: Biophysics. Valid until : 04/06/2030.

2012 NOFYSAS 2012 - Individual Research Grants for young researchers.
International School for Advanced Studies - SISSA - Trieste (Italy)

2010 **Qualification aux fonctions de Maître de Conférences**
Qualified for applying to positions in French Universities as an Assistant Professor
Fields : Condensed Matter Physics (sector 28) and Biochemistry&MolecularBiology (sector 64).

2010 Post-doctoral fellowship, *Ecole Normal Supérieure, Paris*

Stages and Schools

2011 **School of Pure and Applied Biophysics**
Subject: Protein Stability and Pathways of Self-Assembly
Venice, Italy, January 24-28.

2007-2008 **Visiting Scientist at NIST Center for Neutron Research**
NIST, Washinghton DC, USA, July 2007 et Mars 2008.

2006 **[PhD]Internship in Protein Biochemistry**
Deuteration Laboratoiry, **ILL/EMBL**, Grenoble, May-October 2006.
Expression and purification of the protein IF6 isolated from *M.Jannaschii* et du *S. cerevisiae*.
Supervisors: Michael Haertlein and Trevor Forsyth

2006 **CCP5 and Marie Curie Actions: Methods in Molecular Simulation Summer School**
University of Cardiff, Wales, United Kingdom.
Session: Simulation of Organic and Bio-Molecules
(Lectures and Practicals)

2006 **Higher European Research Course for Users of Large Experimental Systems** (H.E.R.C.U.L.E.S.)
ESRF and ILL, Grenoble, France and ELETTRA Synchroton, Trieste, Italy
Session: Neutron and Synchrotron Radiation for Biomolecular Structure and Dynamics
(Lectures, Tutorials and Practicals.)

2005 **Short Internship in Bioinformatics**
Université Pierre et Marie Curie (Paris VI), Paris.
Session: Algorithms and statistical bases for sequence analysis.
Supervisor: Joel Pothier.

2001-2002 **Undergraduate Practical Training**
Centre de Biophysique Moléculaire (CBM) - CNRS Orleans
Subject: Relaxation process in biomolecules by molecular simulation and signal analysis.
Supervisors: Prof. G. Kneller and K. Hinsen.

Teaching

2019-2020 Tutorials of Physics I (mechanics), University of Rome ”Tor Vergata”, Dept. Engineering (30hours).

2019-2020 University of Rome ”Tor Vergata”, Dept. Engineering. Lessons and tutorials on basic mathematics for first-year students (160 hours).

2016 Winter school ”SMART 2015 - Space-time Multiscale Approaches for Research and Technology”
Scuola Normale di Pisa, 25-29 January 2016
Tutorials.

2010-2011 Université Paris Nord - Teaching assistant
48h Tutorials- Physics: Mechanics - Undergraduates in Biochemistry and Biology
20h Practical works- Physics: Optics and Waves - Undergraduates in Biochemistry and Biology

Université Paris Descartes - Teaching assistant
17h Tutorials- Physics: Waves - Undergraduates in Biomedical Science
20h Pratical works- Physics: Optics and Waves - Undergraduates in Biomedical Science
30h Tutorials- Physics: Ray Optics - Undergraduates in Biomedical Science

Research

My research activity is focused on the study of structural and dynamic properties of proteins implemented through a combination of experimental and computational methodologies. In recent years, I have focused my studies on two main strands: the development of theoretical and computational methods for a more effective interpretation of experimental data and the use of computational techniques for the study of ligand-protein interactions and the identification of possible protein inhibitors under pathogenic conditions. More recently, my work has focused on the use of different computational approaches to characterize the allosteric regulatory mechanism of SHP2 phosphatase, a multidomain protein involved in several types of cancer and some rare genetic diseases.

The topics that have shaped my research activities mainly include:

1. Structural properties and dynamics of protein-ligand complexes
2. Computational methods for structural dynamics analysis of proteins.
3. Theoretical models for protein dynamics analysis based on neutronic diffusion and NMR data.
4. Protein dynamics under extreme thermodynamic conditions
5. Theoretical models for characterizing the secondary structure of proteins

Bibliometrics

H-index : 13
Citations : 672
Last update : 10/2022 (Google Scholar)

Publications

Articles in "peer-review" journals[1]

2021 **Calligari P**, Santucci V, Stella L, Bocchinfuso G. "Discriminating between competing models for the allosteric regulation of oncogenic phosphatase SHP2 by characterizing its active state", *Comp. Struct. Bio. J.*, doi: 10.1016/j.csbj.2021.10.041 (in press).

Bobone S, Pannone L, Biondi B, Solman M, Flex E, Canale VC, **Calligari P**, *et al., and Stella L. "Targeting Oncogenic Src Homology 2 Domain-Containing Phosphatase 2 (SHP2) by Inhibiting Its Protein–Protein Interactions",* J. Med. Chem.*, ASAP doi:10.1021/acs.jmedchem.1c01371*

2020 *Polovitskaya MM, Barbini C, Martinelli D, Harms FL, Sessions Cole F,* **Calligari P***, Bocchinfuso G, Stella L, Ciolfi A, Niceta M,* et al. *"A Recurrent Gain-of-Function Mutation in CLCN6, Encoding the ClC-6 Cl−/H+-Exchanger, Causes Early-Onset Neurodegeneration",* Amer. J. Hum. Gen.*,* **107** *(6), 1062-1077.*

Gioia M, Ciaccio C, **Calligari P***, De Simone G, Fasciglione GF, di Masi A, Di Pierro D, Bocedi A, Ascenzi P, Coletta M. Role of proteolytic enzymes in the COVID-19 infection and promising therapeutic approaches,* Biochemical Pharmacology*,* **182***,114225.*

Anselmi M, **Calligari P***(co-first authors), Hub J, Tartaglia M, Bocchinfuso G, Stella L. "Structural Determinants of Phosphopeptide Binding to the N-Terminal Src Homology 2 Domain of the SHP2 Phosphatase,* Journal of Chemical Information and Modelling*,* **60** *(6), 3157–3171.*

Calligari P*, Bobone S, Ricci G, Bocedi A. Molecular investigation of Covid-19 proteins and their interactions with antiviral drugs.* Viruses*, 12(4), 445.*

Martinelli S., Pannone L., Lissewski C., Brinkmann J., Flex E., Schanze D., **Calligari P.***, Anselmi M., Pantaleoni F., Canale, V.C., Ioannides A., Rahner N., Josifova D., Bocchinfuso G., Stella L., Ryten M., Tartaglia M., Zenker M., Pathogenic PTPN11 variants involving the poly-glutamine Gln255-Gln256-Gln257 stretch highlight the relevance of helix B in SHP2's functional regulation.* Human Mutation*, 41,6,1171-1182.*

• **Calligari P***, Torsello M, Bortoli M, Polimeno A and Orian L. Modelling of* Ca^2*-promoted structural effects in wild type and post-translationally modified Connexin26.* Molecular Simulation*, 46 (3), 235-245.*

2019 *Keshavan S,* **Calligari P***, Stella L, Fusco L, Delogu L, Fadeel B. Nano-bio interactions: a neutrophil-centric view,* Cell Death & Disease*, 10:569.*

Varnava K G, Mohid Sk. A, **Calligari P***, Stella L, Reynnison J, Bhunia A, and Sarojini V. Design, Synthesis, Design, Synthesis, Antibacterial Potential, and Structural Characterization of N-Acylated Derivatives of the Human Autophagy 16 Polypeptide,* Bioconjugate Chem*, 30, 7, 1998-2010.*

2018 *Tuan Tran A, Sadet A,* **Calligari P***, Lopes P, Ouazzani J, Sollogoub M, Miclet E and Abergel A., Targetting the Pentose Phosphate Pathway: characterization of a new 6PGL inhibitor.* Biophysical J.*,* **115***, 1-13.*

Bauer CK, **Calligari P***, Radio FC, Caputo V, Dentici ML, Falah N, High F, Pantaleoni F, Barresi S, Ciolfi A, Pizzi S, Bruselles A, Person R, Richards S, Cho MT, Claps Sepulveda DJ, Pro S, Battini R, Zampino R, Digilio MC, Bocchinfuso G, Dallapiccola B, Stella L, Tartaglia M. Gating-affecting mutations in kcnk4 cause a recognizable neurodevelopmental syndrome.* Am. J. Human Gen.*,* **103***(4), 621-630.*

Mukherjee S, Bondarenko O, Kohonen P, Andón F, Brzicová T, Gessner I, Mathur S, Bottini M, **Calligari P***, Stella L, Kisin E, Shvedova A, Autio R, Salminen-Mankonen H, Lahesmaa R, and Fadeel B. Macrophage sensing of single-walled carbon nanotubes via Toll-like receptors.* Scientific Reports*,*

[1] The symbol • indicates works in which I was a "corresponding author".

8:1115.

2017 *Gerolin, M.; Zerbetto, M.; Moretto, A.; Formaggio, F.; Toniolo, C.; van Son, M.; Shabestari, M.; Huber, M.;* **Calligari P.***; Polimeno, A. An Integrated Computational Approach to the Electron Paramagnetic Resonance Characterization of Rigid* 3_{10}*-Helical Peptides with TOAC Nitroxide Spin Labels,* J. Phys. Chem. B*,***121** *(17), 4379-4387.*

• **Calligari PA***, Gerolin M, Abergel D, Polimeno A. Decomposition of Proteins into Dynamic Units from Atomic Cross-Correlation Functions,* J Chem Theor and Comp*, 2017, 13 (1), pp 309-319.*

2015 • **Calligari PA***, Calandrini V, Ollivier J, Artero JB, Haertlein M, Johnson M, Kneller GR. Adaptation of Extremophilic Proteins with Temperature and Pressure: Evidence from Initiation Factor 6,* J Phys Chem B*, 2015 Jun 25;119(25):7860-73.*

2014 • **Calligari P** *and Abergel D, Multiple Scale Dynamics in Proteins Probed at Multiple Time Scales through Fluctuations of NMR Chemical Shifts,* J. Phys. Chem. B*,* **118***(14):3823–31.*

2012 **Calligari P** *and Abergel D, Towards the characterization of fractional stochastic processes underlying methyl dynamics in proteins.* J. Phys. Chem. B*,* **116***(43):12955–12965.*

Calligari P.A. *and Kneller G.R., ScrewFit: Combining localization and description of protein secondary structure.*Acta Crystallographica D*,* **68***, 1690–1693.*

Kneller, G.R., Hinsen, K. and **Calligari, P.***, A minimal model for the diffusion-relaxation backbone dynamics of proteins.* J. Chem. Phys.*,* **136***, 191101 -* COVER ARTICLE*.*

Calligari P.A.*, Salgado G.F., Pelupessy P., Lopes P., Ouazzani J., Bodenhausen G. and Abergel, D., Insights into internal dynamics of 6-Phosphogluconolactonase from Trypanosoma brucei studied by NMR and Molecular Dynamics,* Proteins: Structure, Function, and Bioinformatics*,* **80***(4), 1196-1210.*

2011 **Calligari P.A.***, Calandrini V., Kneller G., Abergel D., From NMR Relaxation to Fractional Brownian Dynamics in Proteins : Results from a Virtual Experiment,* J. Phys. Chem. B*,* **115***(43):12370-9.*

Chevrot G., **Calligari P.***, Hinsen K., and Kneller G.R., Least constraint approach to the extraction of internal motions from molecular dynamics trajectories of flexible macromolecules,* J. Chem. Phys.*, 135, 084110.*

2009 • **Calligari P.A.***, Kneller G.R., Giansanti A., Ascenzi P., Porrello A., Bocedi A. Inhibition of viral group-1 and group-2 neuraminidases by oseltamivir: a comparative structural analysis by the ScrewFit algorithm.* Biophysical Chemistry*,* **141***(1), 117-123.*

2008 *Calandrini V., Hamon V., Hinsen K.,* **Calligari P.***, Bellisent-Funel M.-C. and Kneller G.R., Relaxation dynamics of lysozime in solution under pressure: combining molecular dynamics and quasielastic neutron scattering.* Chemical Physics*,* **345***, 289-297.*

2006 *Hamon V.,* **Calligari P.***, Hinsen K., Kneller G.R. Simulation studies of structural changes and relaxation processes in lysozyme under pressure,* J. of Non-Crystalline Solids*,* **352***, 4417-4423.*

Kneller G.R. and **Calligari P.***, Efficient characterisation of protein secondary structure in terms of screw motions.* Acta Crystallographica **D62***, 302-311, (2006) -* COVER ARTICLE*.*

Monografie - contributi con sistema di ”peer-reviewing”

2011 *Calandrini V., Pellegrini E.,* **Calligari P.***, Hinsen K., Kneller R.G., nMoldyn - Interfacing spectroscopic experiments, molecular dynamics simulations and models for time correlation functions, Collection SFN,* **12***, 201-232. doi: http://dx.doi.org/10.1051/sfn/201112010.*

2010

M.R. Johnson, M. Zbiri, M.A. Gonzalez, E. Pellegrini, **Calligari, P.**, *L. Capogna, E. Farhi, A. Filhol, R. Ghosh et D. Richard, Diffusion inélastique des neutrons et simulations atomistiques, Collection SFN,* **10***, 427-447. doi: 10.1051/sfn/2010007 .*

Other publications

2019 **Conference Abstract :** *Radio, F. C., Calligari, P., Caputo, V., Dentici, M. L., Falah, N., High, F.,* et al. *Gating-affecting mutations in KCNK4 cause a recognizable neurodevelopmental syndrome. European Journal of Human Genetics, 27, 504-1504).*

2018 **PDB entry :** *Structure 5ZYX: Solution NMR structure of K30 peptide in 10 mM dioctanoyl phosphatidylglycerol (D8PG) DOI: 10.2210/pdb5ZYX/pdb*