Curriculum Vitae et Studiorum
for GIORGIO COLOMBO

PERSONAL DATA

Full Name: Giorgio Colombo
Google Scholar: https://scholar.google.it/citations?user=-vCLX9kAAAAJ&hl=en
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Researcher ID: http://www.researcherid.com/rid/A-2730-2012

Date of Birth: June 24, 1971
Place of Birth: Monza, Italy

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EDUCATION

Academic Year 94/95 Laurea (Masters Degree) in Chemistry at the University of Milano (Final Grade 110/110)

1996-99 Works towards his Ph.D. dissertation on *Structure, Reactivity and activity of proteases: computational studies* under the direction of Prof.s Scolastico and Carrea

Jan 1998-Jan 99 Visiting scientist in Ken Merz's laboratory at Penn State University as part of his doctoral training. Works on the use of mixed Quantum/Molecular mechanics methods to describe the reactivity of enzymes in solution and on the application of molecular dynamics to the study of stability-activity relationships of proteins.

Feb 2000 PhD at the University of Milano

PROFESSIONAL EXPERIENCE

December 2013	Appointed member of the Scientific and Technical Board of the Italian National Association for Cancer Rsearch (AIRC).
December 2013	- National Habilitation (Abilitazione Scientifica Nazionale) as a Full Professor in in Organic Chemistry (Professore di Prima Fascia, Chimica Organica). - National Habilitation (Abilitazione Scientifica Nazionale) as a Full Professor in Models and Methodologies for Chemical Sciences (Professore di Prima Fascia, Modelli e Metodologie per le Scienze Chimiche) - National Habilitation (Abilitazione Scientifica Nazionale) as a Full Professor in General and Clinical Biochemistry (Professore di Prima Fascia, Biochimica Generale e Biochimica Clinica)
May 2001-Present	Founder and Head of the Computational Biochemistry Group at ICRM-CNR, Milano.
Dec 1999-Apr 2001	Post-doctoral research associate in Prof.s Alan Mark and Herman Berendsen laboratories at the University of Groningen, working on protein folding simulations, and membrane protein simulations. Teacher in the course of Biophysics for graduate and undergraduate students.
May 2001	Research scientist at the CNR "Istituto di Chimica del Riconoscimento Molecolare" in Milano, where he started up and currently runs the computational biochemistry group.

FELLOWSHIPS AND AWARDS

December 1999	Recipient of a Training and Mobility Research Programme (TMR) fellowship by the European Community (EC)
December 2000	Recipient of a Marie Curie Fellowship from the European Community commission
November 2004	Recipient of the Young Investigator Award from the Division of Biological Systems of the Italian Chemical Society
December 2008	Recipient of the Career Award from the President of Lombardy Region.

ABROAD EXPERIENCE

January 1998-January 1999	At the Pennsylvania State University (State College, PA, USA) in the Group of Prof. Ken Merz.

December 1999-April 2001	At the Biophysical Chemistry Department, University of Groningen (Groningen, The Netherlands) in the Group of Prof. Alan E. Mark and Herman Berendsen.
2005	Visiting Scientist at the Department of Physiology and Biophysics, Mount Sinai School of Medicine, New York, NY, USA.
June-July 2013	Visiting Professorship at the Department of Biochemistry and Biophysics of the University of California at San Francisco (UCSF). Host David. A. Agard.

TEACHING AND TUTORING EXPERIENCE

- Contract professor for the "Organic Chemistry" course at the faculty of Medical Biotechnology, Università Vita e Salute San Raffaele, Milano, year 2016/2017
- Contract professor for the course "Molecular Simulations of Biochemical Systems", SISSA-ISAS Trieste, years 2011-2016.
- Professor for the masters course "Drug Design and Development", Faculty of Pharmacy, University of Coimbra, year 2013-2014.
- Appointed as contract professor for the "Bioinformatics" course at the faculty of Biotechnology, University of Milano, year 2004.

Taught several graduate and undergraduate courses in biophysics, computational chemistry and computational biology at the graduate and undergraduate level:

- Ph.D. school in Soft-Condensed Matter and Physics and Chemistry of Biological Systems at SISSA-ISAS Trieste (Italy)
- Ph.D. school in Molecular Medicine at IRCCS Candiolo (Italy)
- Ph.D. school in Bioengineering at Politecnico di Milano (Italy)
- Ph.D. school in Chemical Sciences at the University of Milano (Italy)
- T.A. in the "Moleculaire herkenning" (Molecular Recognition) course at the University of Groningen (Holland)

Summer and Graduate Schools

- Invited speaker at the "3rd Edition of the Summer School of Integrative Molecular and Cellular Biology (UIMP-CSIC)", Santander (Spain), 29th August - 1st September 2016.
Title of the Lecture: Protein stability and functional dynamics: Ligand binding, allostery and protein-protein interactions

- Invited speaker at the XXXVII edition of the "Attilio Corbella" Summer School on Organic Synthesis.

Gargnano (BS), Italy, 18-22nd June 2012.
Title of the Lecture: Computational Design of New Biomolecules for Organic Chemistry

- Invited speaker at the Winter School in Physical Organic Chemistry, Brixen (Italy), 11-18th January 2007.
Title of the lesson: Molecular Dynamics Simulations of Biological Systems.

- Invited speaker and organizer of the Molecular Dynamics session of the "School of Computational Chemistry", Siena (Italy) 25-29th September 2006.
Title of the lesson: Molecular Dynamics Simulations of Biological Systems.

- Invited Speaker at the *International Summer School: Advanced Modeling of Biological Function,* August 7th-13th 2004, International University of Bremen, Germany.
Title of the Lecture: The investigation of Biomolecular Systems: What an Simulations Tell Us?

Dr. Colombo has been and currently is the supervisor of several master and Ph.D. students.

Supervisor of Masters Theses

- 2003-2004. Studies of the folding and aggregation of peptides via MD simulations. Candidate Fabio Simona, Physics Masters - Università Statale di Milano.

- 2004-2005. The determinants of stability in the human prion and doppel protein: insights into folding and misfolding from the analysis of the stabilization energy distribution in different conditions. Candidate Stefano Nicola Colacino, Physics Masters - Università Statale di Milano.

- 2004-2005. Evaluation of GAG-chain sliding through molecular mechanics methods. Candidate Emanuele Bianchi Janetti, Engineering Bachelor (Laurea Triennale) – Politeccnico di Milano.

- 2005-2006. Molecular simulations for the study of protein-nucleotide interactions. Candidate Isabella Gambini, Engineering Bachelor (Laurea Triennale) – Politeccnico di Milano.

- 2007-2008. Protein dynamics and stability: implications for the design of polypeptidic sequences. Candidate Chiara Baragli, Chemistry Bachelor (Laurea Triennale) - Università Statale di Milano.

- 2011-2012. Discovery of leads for the treatment of angiogenesis using integrated computational approaches. Candidate Giulia Pagani, Bioinformatics Masters (Laurea Specialistica) - Università di Milano Bicocca.

- 2016-2017. A structural vaccinology approach to *Burkholderia Pseudomallei* antigen redesign. Candidate Marco Amabili, Chemistry Masters (Laurea Specialistica) - Università Statale di Milano.

- 2018-2019. Computational approaches to treating neurodegenerative disease. Candidate Marta Maroni, Chemistry and Pharmaceutical Technology Masters (Laurea Specialistica) - Università di Pavia

- 2019-2020. Integrative structural modeling of MusK. Candidate Manfredi Alberti, Biotechnology Masters (Laurea Specialistica) – Università di Pavia

- 2019-2020. Modeling G-Quadruplex-inhibitor interactions in HIV-1 genome as antiviral strategy. Candidate Matteo Castelli, Chemical Sciences Masters (Laurea Specialistica) – Università di Pavia

- 2020-2021. Development of PPI inhibitors targeting Hsp90 Complexes. Luca Torielli, Chemistry and Pharmaceutical Technology Masters – Università di Pavia

- 2020-2021. Blocking CypD-TRAP1 interactions. Beatrice Pavesi, Biology and Biotechnology Bachelor – Università di Pavia

- 2021-2022. Drug Discovery for Light Chain Amyloidosis. Elisa Seghetti, Biology and Biotechnology Bachelor – Università di Pavia

- 2021-2022. Investigation of a conserved cryptic site in the SARS-CoV-2 Spike Protein among Variants of Concern: computational methods to design new active ligands. Elena Frasnetti, Chemical Sciences Masters (Laurea Specialistica) – Università di Pavia

- 2021-2022. Targeting the Hsp90:p23:GR maturation complex *in silico*: from the study of the internal dynamics to the design of modulators of interactions. Andrea Magni. Chemical Sciences Masters (Laurea Specialistica) – Università di Pavia

- 2023-2024: Deep APBS: a novel convolutional neural network for druggable sites prediction. Beattice Pavesi. Pharmaceutical and Medical Biotechnologies Masters (Laurea Specialistica) – Università di Pavia

<u>Supervisor of PhD Theses</u>

- 2001-2004. Supervisor of the thesis: Protein folding and protein stability: a molecular dynamics perspective. Candidate Giacomo M.S. De Mori, PhD school in Chemical Sciences - Università Statale di Milano.

- 2002-2005. Supervisor of the thesis: Biomolecular simulations by classical dynamics. Candidate Stefano Pieraccini, PhD school in Chemical Sciences - Università Statale di Milano.

- 2003-2006. Supervisor of the thesis: Molecular dynamics simulations of molecular recognition in biological processes. Candidate Massimiliano Meli, PhD school in Chemical Sciences - Università Statale di Milano.

- 2004-2008. Supervisor of the thesis work of Marco André Coelho das Neves, Faculdade de Farmacia, Universidade de Coimbra (Portugal). Title: Aromatase inhibitors in breast cancer: the discovery of new compounds by computational design and biochemical evaluation.

- 2007-2010. Supervisor of the thesis: Molecular dynamics simulations of biological macromolecules: applications to structural vaccinology and peptide design. Candidate Guido Scarabelli, PhD school in Chemical Sciences - Università Statale di Milano.

- 2012-present, Supervisor of the PhD thesis work of Maria Armandina Cruz de Jesus Baptista, Faculdade de Farmacia, Universidade de Coimbra (Portugal).

- 2012-2015. Supervisor of the thesis: Investigating and predicting the determinants of protein protein interactions through computational-structural biology approaches: implications for structural vaccinology. Candidate Claudio Peri, PhD School in Biological and Molecular Sciences - Università Statale di Milano.

- 2014-2017. Supervisor of the thesis: Computational modeling of proteins: from statistical mechanics to immunology. Candidate Riccardo Capelli, PhD School in Physical Sciences - Università Statale di Milano.

- 2018-2021. Supervisor of the thesis: Computational approaches to targeting PPIs in functional complexes. Candidate Filippo Marchetti, PhD School in Chemical Sciences - Università Statale di Milano.

- 2020-2023. Supervisor of the thesis: Computational approaches to model Hsp90 complexes in cancer. Candidate Matteo Castelli, PhD School in Chemical Sciences - Università di Pavia.

- 2020-2023. Supervisor of the thesis: Experimental and computational approaches to a pan-coronavirus strategy. Candidate Alice Triveri, PhD School in Chemical Sciences - Università di Pavia.

- 2021-2024. Development of allosteric ligands of TRAP1 via theoretical and computational methods. Candidate Luca Torielli, PhD School in Chemical Sciences - Università di Pavia.

- 2022-2025. Studying and Targeting Networks in Chemical Biology with Computer Simulations. Candidate Andrea Magni, PhD School in Chemical Sciences - Università di Pavia.

- 2022-2025. Predicting the biology of small molecules via an integrated structural and chemoinformatic approach. Candidate Elena Frasnetti, PhD School in Chemical Sciences - Università di Pavia.

- 2022-2025. Theoretical models for Protein interactions in health and disease. Candidate Giorgio Bonollo, PhD School in Chemical Sciences - Università di Pavia.

- 2022-2025. AI models for chemistry. Candate Ivan Cucchi, PhD School in Computational Mathematics - Università di Pavia.

- 2023-2026. Computational design of modulators of protein interactions in health and disease. Candidate Cristiano Sciva, PhD School in Chemical Sciences - Università di Pavia.

- 2023-2026. Test and validation of chemical tools for chaperone networks. Candidate Denis Komarov, PhD School in Chemical Sciences - Università di Pavia

Post-Doctoral Supervisor

- 2002-2004. Dr. Luca Monticelli. Dr. Monticelli is now a PI researcher at INSERM, Lyon France.

- 2002-2005. Dr. Massimiliano Meli. Dr. Meli is now a permanent researcher of ICRM-CNR as a research Technician.

- 2004-2005. Dr. Carlos Simoes. Dr. Simoes is now the founder and CTO of BSIM^2, small company for drug design in the Coimbra Area, Portugal.

- 2006-2008. Dr. Elisabetta Moroni. Dr. Moroni is now is now a permanent researcher of SCITEC-CNR as a researcher.

- 2006-2011. Dr. Giulia Morra. Dr. Morra is now a permanent researcher of ICRM-CNR as a researcher.

- 2008-2011. Dr. Alessandro Genoni. Dr. Genoni is now a permanent researcher at CNRS, Nancy, France.

- 2010-2012. Dr. Dario Corrada. Dr. Corrada is now a staff member of Istituto Gonzaga, Milan, Italy.

- 2011-2013. Dr. Jacopo Sgrignani. Dr. Sgrignani is now a senior researcher at IRB, Bellinzona, Switzerland.

- 2012-2016. Dr. Alessandro Gori. Dr. Gori is now a permanent researcher of ICRM-CNR as a researcher.

- 2013-2017. Dr. Antonella Paladino. Dr. Paladino is now a permanent researcher of IBB-CNR.

- 2013-2018. Dr. Silvia Rinaldi. Dr. Rinaldi is now a permanent researcher of ICCOM-CNR Florence as a researcher.

- 2016-2020. Dr. Ilda D'Annessa. Dr. D'Annessa is now a staff member at the company MedTronic.

- 2017-2020. Dr. Mariarosaria Ferraro. Dr. Ferraro is now a permanent researcher at Sosei-Heptares in Cambridge, UK.

- 2018-2019. Dr. Marco Montefiori. Dr. Montefiori works as a senior investigator at Ichnos Sciences .

- 2018-2019. Dr. Enrico Fassi. Dr. Fassi is now a researcher at the University of Milano.

- 2019-present. Dr. Stefano A. Serapian, Now permanent researcher at the University of Pavia

- 2019-present. Dr. Filippo Marchetti, joint collaboration with E4 Computer Company

- 2022-present. Dr. Federica Guarra, AIRC Fellow

- 2022-2023. Dr. Emanuele Casali, HBP Fellow

Thesis Committees

- May 2008. Thesis Committee for the thesis of Florian Sieker, Jacobs University, School of Engineering and Science, Bremen (Germany). Title: Analysis of Peptide binding to MHC class I molecules and the function of tapasin during the binding process.

- November 2010. Thesis Committee for the PhD defense of Andrea Zen, SISSA Trieste.

- February 2011. Thesis Committee for the PhD defense of the candidates of the PhD school in Chemistry, Università Milano Bicocca.

- February 2011. Thesis Committee for the PhD defense of the candidates of the PhD school in Chemistry, Università Milano Bicocca.

- November 2013. Thesis Committee for the PhD defense of Alejandro Panjkovich at the Universitat Autonoma de Barcelona, Spain.

- February 2014. Thesis Committee for the evaluation of PhD Defenses in Chemical Sciences, Università di Milano Bicocca, Milano, Italy.

- September 2014. Thesis Committee for the PhD defense of Tai Wang at the University of Geneva, Switzerland.

- October 2015. Thesis Committee for the PhD defense of Andrea Perez-Villa at SISSA-ISAS Trieste, Italy.

- 2015-present. External advisor and referee for the PhD Thesis of Stefano Motta, PhD Course in Chemical Sciences, Università di Milano-Bicocca.

- October 2016. Thesis Committee for the PhD defense of Luca Ponzoni at SISSA-ISAS Trieste, Italy.

- February 2017. External evaluator and thesis committee for the PhD Course in Chemical Sciences, XXIX Cycle, Università di Roma "Tor Vergata".

- October 2017. Thesis Committee for the PhD defense of Lorenzo Casalino at SISSA-ISAS Trieste, Italy.

- March 2019. Thesis Committee in the PhD evaluation of the PhD in Biotechnology, Chemistry and Pharmacy, University of Siena, Italy.

- November 2019. Thesis Evaluation Committee for the thesis of Francesco Ambrosetti, PhD in Life Sciences, University of Tor Vergata, Rome, Italy

- December 2021. Thesis Evaluation Committee for the thesis of Mukesh Kumar, PhD in the School of Health and Medical Sciences, University of Copenhagen, Copenhagen, Denmark

- February 2022. Thesis Evaluation Committee for the thesis of Crescenzo Coppa, PhD in Chemical Sciences, University of Milano, Milano, Italy

- February 2024. Thesis Examiner for the thesis of Anna Katerina Antonovic, PhD candidate in the School of Physical and Chemical Sciences, Queen Mary University London, UK

- February 2024. Thesis Evaluation Committee for the thesis of Michele Gandolfi, PhD in Chemical Sciences, University of Milano, Milano, Italy

REFEREE ASSISTANCE FOR JOURNALS and FUNDING BODIES

Dr. Colombo is a Member of the Editorial Board of

- Frontiers in Molecular Biosciences
- Chemistry - Open

Reviewer Duties for Scientific Journals

- Nature Chemical Biology
- Nature Communications

- eLife
- Cell
- Journal of the American Chemical Society
- Biochemistry
- Journal of Physical Chemistry
- Journal of Molecular Biology
- Journal of Organic Chemistry
- Biophysical Journal
- Proteins: structure, function and bioinformatics
- Journal of Molecular Modeling
- Biophysical Chemistry
- Molecular Simulations
- Structure
- Accounts of Chemical Research
- Journal of Chemical Physics
- Journal of Physical Chemistry Letters
- Chemical Science

Reviewer/Panel Member Duties for Funding Agencies and Scientific Societies

- Israel Science Foundation
- Reviewer for the 7th Framework Programme of the European Community
- ICREA (Spain)
- AICR (Scotland)
- ANR (France)
- KNOW (The Netherlands)
- ERC (European Research Council)
- PRACE (European Union)
- HELMHOLTZ SOCIETY (Germany)
- Consejo Nacional Ciencia y Tecnologia (Mexico)

INDUSTRIAL COLLABORATIONS

2002-2004	Scientific Consultant for “Vicuron S.P.A.” in the field of drug design of new antibiotic molecules.
2002-2003	Scientific Consultant for “Nicox Research Institute S.r.l.”
2007	Scientific Consultant for “EOS, Ethical Oncology Science, Milano”
2009 - 2012	Scientific Consultant for “Kemotech S.r.l”
2019	Scientific Consultant for “3V Sigma”.
2021-2023	E4 Scientific Computing

2023	Nerviano Medical Sciences
2022-2024	Cohen Pharma, LTD

MEMBERSHIPS AND DUTIES FOR SCIENTIFIC SOCIETIES

June 2010-2014	Elected Councilor of the International Society for Quantum Biology and Pharmacology (ISQBP)
2005 - 2015	Elected Board Member of the Division of Chemistry For Biological Systems of the Italian Chemical Society
Since 2004	Member of the International Society for Quantum Biology and Pharmacology

LANGUAGES

Italian (mother tongue), English (Fluent), Dutch (basic knowledge), Spanish (basic knowledge)

COMPUTER SKILLS

Operating Systems:	Linux, Unix, Windows, Mac-OSX Set up and management of HPC cluster
Programming Languages:	C, Fortran
Known Programs:	Biochemical Systems Simulation: AMBER, MAESTRO, GROMACS Gaussian94, UCSF-Chimera

MAIN GRANTS

- **Title of the project:** Thrombospondin-1 domains affecting angiogenesis and tumour behaviour: Identification and therapeutic exploit.
  Funding Organization: Italian Association for Cancer Research (AIRC).
  Duration: 2004-2007
  Role in the project: Head of operating unit, Co-PI
  Funding received: 75000€
  Contract number: AIRC-1281

- **Title of the project:** Folding and aggregation of proteins: Metals and Biomolecules in Conformational diseases.
  Funding Organization: MIUR – FIRB
  Duration: 2004-2007

Role in the project: Head of operating unit, Co-PI
Funding received: 70000€
Contract number: MIUR-FIRB RBNE03PX83

- **Title of the project:** Combining biophysics, bioinformatics and chemical biology for the discovery of new antineoplastic molecules based on endogenous inhibitors of angiogenesis.
  Funding Organization: Ministry of Health – Young Investigator Award
  Duration: 2009-2012
  Role in the project: Coordinator
  Funding received: 504000€
  Contract number: GR 2007-683210r

- **Title of the project:** Rational design of antineoplastic molecules based on endogenous inhibitors of angiogenesis.
  Funding Organization: Italian Association for Cancer Research (AIRC).
  Duration: 2008-2010
  Role in the project: Head of operating unit, Co-PI
  Funding received: 75000€
  Contract number: AIRC-5606

- **Title of the project:** New integrated strategies for the discovery of antineoplastic molecules based on endogenous inhibitors of angiogenesis: from computational biology and biophysics to functional biology in vivo and in vitro
  Funding Organization: Cariplo Foundation
  Duration: 2008-2011
  Role in the project: Coordinator
  Funding received: 313000€
  Contract number: 2008.2198

- **Title of the project:** Targeted therapy by blocking protein hubs: Rational Discovery of New Heat Shock Protein 90 Inhibitors
  Funding Organization: Italian Association for Cancer Research (AIRC)
  Duration: 2009-2012
  Role in the project: Principal Investigator.
  Funding received: 150000€
  Contract number: MFAG-5890

- **Title of the project:** From Genome to Antigen: An integrated approach to vaccine development,
  Funding Organization: MIUR-PRIN 2008
  Duration: 2010-2012
  Role in the project: Head of operating unit, Co-PI
  Funding received: 12000€
  Contract number: MIUR 2008K37RHP_002

- **Title of the project:** From Genome to Antigen: a Multidisciplinary Approach towards the Development of an Effective Vaccine Against Burkholderia pseudomallei, the Etiological Agent of Melioidosis
  Funding Organization: Cariplo Foundation
  Duration: 2010-2013
  Role in the project: Head of operating unit, Co-PI
  Funding received: 225000€
  Contract number: 2009-3577

- **Title of the project:** New Integrated Strategies for Vaccine Design
  Funding Organization: Lombardy Region
  Duration: 2010-2012
  Role in the project: Coordinator
  Funding received: 150000€
  Contract number: SAL-45

- **Title of the project:** Integrating computational biology with medicinal chemistry to discover new mechanism-based Hsp90 inhibitors
  Funding Organization: Italian Association for Cancer Research (AIRC)
  Duration: 2011-2014
  Role in the project: Principal Investigator.
  Funding received: 240000€
  Contract number: IG11775

- **Title of the project:** Flagship project *Interomics*
  Funding Organization: MIUR-CNR GRANT
  Duration: 2012-2015
  Role in the project: Head of operating unit, Co-PI.
  Funding received: 300000€
  Contract number: CNR-PB05

- **PERSONAL AWARD FROM THE CARIPLO-UNESCO CALL** "*Exploration of new research frontiers – Award 2011"*. Title of the project: Chemical control of signalling pathways by modulation of hub proteins (**Checosp**), **230 K€.** Special call for funding dedicated to International year of Chemistry 2011.
  The selection committee was composed by: - **Aaron Ciechanover**, Technion- Israel Institute of Technology, Nobel Laureate for Chemistry 2004; - **Gerhard Ertl**, Fritz-Haber Institut Max-Planck, Nobel Laureate for Chemistry 2007 - **Oliver Guthmann**, Investment Manager of BASF Venture - **Krzysztof Matyjaszewski**, Carnegie Mellon University, Wolf Prize for Chemistry 2011- **Phillip Szuromi**, Supervisor Senior Editor of Science Magazine.
  Contract number: 2011.1800

- **Title of the project:** DISCOVERY/DEVELOPMENT OF DIAGNOSTIC PROBES AND VACCINE CANDIDATES TARGETING BURKHOLDERIA INFECTIONS

Funding Organization: Region of Lombardy-Cariplo Foundation
Duration: 2013-2015
Role in the project: Coordinator.
Funding received: 651790€ (of which 197000€ to the Colombo Group)
Contract number: 42666248 (2013-0349)

- **Title of the project:** Discovery of selective modulators of the functional dynamics of Hsp90 family members as novel anticancer compounds
  Funding Organization: Italian Association for Cancer Research (AIRC)
  Duration: 2015-2018
  Role in the project: Principal Investigator.
  Funding received: 296000€
  Contract number: IG15420

- **Title of the project:** Epitope grafting on bacterial vesicles to develop a novel Burkholderia vaccine. (acronym: EGV)
  Funding Organization: Italian Ministry of Research and University.
  Duration: 2017-2019
  Role in the project: Co-PI
  Funding: 66000€
  Contract number: 2015JTL4HL

- **Title of the project:** Integrative approaches to target Hsp90 complexes in cancer
  Funding Organization: Italian Association for Cancer Research (AIRC)
  Duration: 2018-2022
  Role in the project: Principal Investigator.
  Funding received: 495000€
  Contract number: IG20019

- **Title of the project:** Network REgionAle per lo sviluppo di metodi Diagnostici in risposta rapida a epidemie emergenti e bioemergenze (READy)
  Funding Organization: Lombardy Region
  Duration: 2018-2020
  Role in the project: Co-PI.
  Funding received: 180000€

- **Title of the project:** Identifying and targeting metabolic liabilities in the crosstalk between childhood B-cell lymphomas and their microenvironment
  Funding Organization: IRP
  Duration: 2021-2024
  Role in the project: Co-PI.
  Funding received: 60000€

- **Title of the project:** TRAPping tumor growth: designing molecules to perturb the chaperone TRAP1, from enzymatic activities to cell-cell interaction.
  Funding Organization: Miur
  Duration: 2022-2025
  Role in the project: PI.
  Funding received: 662400€ - 247458€

- **Title of the project:** Development of antineoplastic drug candidates hijacking the cellular folding machinery.
  Funding Organization: AIRC
  Duration: 2023-2027
  Role in the project: PI.
  Funding received: 601000€

- **Title of the project:** IMMUNO-HUB.
  Funding Organization: Ministero della Salute
  Duration: 2022-2026
  Role in the project: Co-PI.
  Funding received: 150000€

INTERNATIONAL and EU GRANTS

- **Title of the project:** Assessment of Structural Requirements in Complement-Mediated Bactericidal Events: Towards a Global Approach to the Selection of New Vaccine Candidates.
  Funding Organization: European Union FP6, SME-STREP research project
  Duration: 2006-2009
  Role in the project: Head of operating unit
  Funding received: 240000€
  Contract number: LSHB-CT-2006-03732

- **Title of the project:** Understanding the Molecular Determinants of Amyloid Fibril Formation in Human Degenerative Diseases.
  Funding Organization: ITALY-QUEBEC INTERNATIONAL PROJECT, joint ministries
  Duration: 2006-2008
  Role in the project: Coordinator
  Funding received: 70000€
  Contract number: 269/P0152152

- **Title of the project:** CTHSP90-Investigating conformational transitions of Hsp90 by bias-exchange metadynamics.
  Funding Organization: European Union HPC Partnership, PRACE.
  Duration: 2013-2014
  Role in the project: PI and Coordinator
  Funding received: 20000000 CPU hours, equivalent to approximately 400000€ worth of value.

Contract number: 2012071270

- **Title of the project:** Selective perturbation of Hsp90 networks: towards a structure based pharmacogenomic approach to personalized drugs.
  Funding Organization: Joint Italian-Israel Bilateral Scientific Agreement
  Duration: 2016-2018
  Role in the project: Coordinator
  Funding received: 100000€
  Contract number: PERTNET

- **Title of the project:** TRAPping the metabolic adaptations of plexiform neurofibroma.
  Funding Organization: NTAP, Johns Hopkins School of Medicine, USA.
  Duration: 2017-2019
  Role in the project: Co-PI
  Funding: 150000 USD
  Contract number: SAP GRANT 123141

- **Title of the project:** BRAVE - Protecting the brain from COVID-19-mediated neurodegeneration through inflammasome inhibition
  Funding Organization: European Commission – Human Brain Project P1-EBRAINS
  Duration: 2021-2023
  Role in the project: Co-PI.
  Funding received: 112500€

- **Title of the project:** KC210150 – "Targeting the Chaperone-Mediated Folding of CDK4 in Kidney Cancer
  Funding Organization: Department of the Army, US ARMY MEDICAL RESEARCH ACQUISITION ACTIVITY
  Duration: 2022-2023
  Role in the project: PI.
  Funding received: 65000USD

- **Title of the project: EBRAINS 2.0**
  Funding Organization: European Commission
  Duration: 2023-2026
  Role in the project: Co-PI.
  Funding received: 75000€

PUBLICATIONS

* indicates corresponding/senior/co-last authorship, when G. Colombo is not first or last author.

H-index 56, Source Google Scholar

(236) Buchner, J.; Alasady, M. J.; Backe, S. J.; Blagg, B. S. J.; Carpenter, R. L.; **Colombo, G**.; Gelis, I.; Gewirth, D. T.; Gierasch, L. M.; Houry, W. A.; et al. Second international symposium on the chaperone code, 2023. *Cell Stress and Chaperones* **2024**, *29* (1), 88-96. DOI: https://doi.org/10.1016/j.cstres.2024.01.003.

(235) Castelli, M.; Magni, A.; Bonollo, G.; Pavoni, S.; Frigerio, F.; Oliveira, A. S. F.; Cinquini, F.; Serapian, S. A.; **Colombo, G.** Molecular mechanisms of chaperone-directed protein folding: Insights from atomistic simulations. *Protein Science* **2024**, *33* (3), e4880. DOI: https://doi.org/10.1002/pro.4880 (acccessed 2024/02/26).

(234) Pasala, C.; Sharma, S.; Roychowdhury, T.; Moroni, E.; **Colombo, G.**; Chiosis, G. N-Glycosylation as a Modulator of Protein Conformation and Assembly in Disease. In *Biomolecules*, 2024; Vol. 14.

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BOOK CHAPTERS

Morra, G.; **Colombo, G.** Understanding allostery to design new drugs. In *Molecular Simulations in Drug Discovery*, a book of the series *Method and Principles in Medicinal Chemistry* published by Wiley-VCH, **2019**

Rinaldi, S.; **Colombo, G.** Designing Chemical Tools with Computational Chemistry. In *Computational Tools for Chemical Biology 2017*, Chapter 3, 69-87 ROYAL SOCIETY OF CHEMISTRY doi: 10.1039/9781788010139

Claudio Peri, Oscar C. Solé, Dario Corrada, Alessandro Gori, Xavier Daura and **Giorgio Colombo** Prediction of antigenic B and T cell epitopes via Energy Decomposition analysis. Description of the web-based prediction tool BEPPE. *Methods in Molecular Biology.* **2015** *In press*

Colombo, G. Computational Design of New Biomolecules for Organic Chemistry. In *Seminars in Organic Chemistry, XXXVII Summer School 'E. Corbella', Società Chimica Italiana Editor,* **2012,** pp. 32-64.

Shea, J.-E.; **Colombo, G.** Inhibiting peptide and protein self aggregation: What can simulations tell us? In *Alzheimer's Disease: Insights into Low Molecular Weight and Cytotoxic Aggregates from In Vitro and Computer Experiments - Molecular Basis of Amyloid-β Protein Aggregation and Fibril Formation;* Derreumaux, P.; Ed.; Molecular Medicine and Medicinal Chemistry; Imperial College Press: London, UK, **2012**; Vol 7. Pp. 401-438, 2013. ISBN: 978-1-84816-754-4.

Morra, G.; Genoni, A.; **Colombo, G.** Protein dynamics and drug design: the role of molecular simulations. In *Protein-Protein Complexes – Analysis, Modeling and Drug Design. Ed. Martin Zacharias.* Imperial College Press. **2010;** ISBN 978-1-84816-338-6

Meli, M. and **Colombo, G.** Molecular simulations of peptides: a useful tool for the development of new drugs and for the study of molecular recognition. In *Peptide Microarrays. Eds. Marina Cretich and Marcella Chiari. Humana Press.* **2009**; ISBN 978-1-60327-393-0

Colombo, G.; Meli, M.; Carrea, G.; Enzyme reactivity studied by Computer simulations. In *Handbook of theoretical and computational Nanotechnology, pp 260-300, Eds. Michael Rieth and Wolfram Schommers, American Scientific Publishers,* **2006.** ISBN 1-58883-048-9

Colombo, G.; Folding and mis-folding of peptides and proteins: Insights from molecular simulations. In *Mem. S.A. It. Suppl. Nr. 4,* **2004**, 24-36

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MOST RELEVANT INVITATIONS AND PRESENTATIONS

Invited seminar at School of Physical and Chemical Sciences, Queen Mary University London, London, UK, 29 February 2024.
Title of the seminar: Studying protein dynamics with an eye to molecular design

Invited speaker at the "2nd International Symposium on Chaperone Code", Alexandria, Virginia, USA, October 26th to 31st 2023.
Title of the seminar: Deciphering the chaperone code with biocomputing.

Plenary Lecture at the "National Meeting of the Division of Chemistry for Biological Systems of the Italian Chemical Society", Milano, Italy, September 27th to 29th, 2023
Title of the seminar: The dynamics of molecular design.

Invited speaker at the "Pharma Summer School 2023", Parma, Italy, September 4th to 29th, 2023.
Title of the seminar: The dynamics of molecular design.

Invited speaker at the "Metabolism Meets Function 4th International Meeting", Bari, Italy, July 21st 2023.
Title of the seminar: Protein dynamics and molecular design: implications for drug and diagnostic development.

Invited seminar at the "Second HBPMolSim Training Workshop on Tools for Molecular Simulation of Neuronal Signaling Cascades", Heidelberg, Germany, 21-23 June 2023.
Title of the seminar: NLRP3 Functional Dynamics: from the Effects of Allosteric Binding to Implications for Drug Design

Invited speaker at the Conference "Structure Based Drug Design, SBDD 2023", Sestri Levante, Italy, 2-4 May 2023.
Title of the seminar: Looking at the jigglings and wigglings of Hsp90 and its partners: from protein dynamics to drug design.

Invited speaker at the Hsp90 World Webinar Series, 6 February 2023.
Title of the seminar: Looking at the jigglings and wigglings of Hsp90 and its partners: from protein dynamics to drug design.

Invited speaker at the "Intensive School of Clinical Bioinformatics", 9th September 2023, Pavia, Italy.
Title of the seminar: Computational Chemistry: epitope prediction and vaccines.

Invited speaker at the Second Virtual International Symposium on Cellular & Organismal Stress Responses, September 8 and 9, 2022.
Title of the seminar: Motions and interactions in Hsp90 and the design of new chemical tools.

Invited speaker at the workshop “Physics of Biomolecules: Structure, Dynamics and Function”, Bressanone, Italy, 5-8 September 2022.
Title of the seminar: How Post-Translational Modifications of a Chaperone Codes for a Switch in Function in the folding machinery: An Atomistic View.

Invited seminar at the Memorial Sloan Kettering Cancer Center, New York, USA, 5 May 2022.
Title of the seminar: Studying protein dynamics with an eye to molecular design: from the discovery of new drugs to applications in immunology and structural vaccinology.

Invited speaker at the CECAM workshop “Quantifying Protein Dynamics and Allosteric regulation in the cell with emerging technologies: From Cryo-EM and NMR to Multiscale Simulations, Networks and Machine Learning”, September 15-17, 2021 Online.
Title of the seminar: Protein dynamics and energy: Implications for ligand design.

Invited speaker at the ACS Spring 2021, April 5-30, 2021. Virtual Seminar Series on “A Call to Action: The Many Roles of Computational Chemistry in Addressing COVID-19”.
Title of the seminar: The answer lies in the energy: how simple atomistic molecular dynamics simulations may hold the key to epitope prediction on the fully glycosylated SARS-CoV-2 spike protein.

Invited speaker at the Workshop “From *in silico* to animal models for the study of human diseases”, Org. University of Aveiro, 17 March 2021.
Title of the seminar: The dynamics of molecular design.

Invited speaker for a Seminar at GSK Pharma & Vaccines, 22 January 2021.
Title of the seminar: The dynamics of molecular design.

Invited speaker for the VALIDATE (Validate.org) Online Seminar Series, 3 December 2020.
Title of the seminar: Computational approaches in structural vaccinology.

Invited speaker at the “Chaperone Code Meeting”, Organized by the State University of New York, Syracuse, 28-29 October 2020.
Title of the seminar: Cracking the chaperone code with computer simulations.

Invited speaker at the “Digital Event - CECAM-ICTP School on Molecular Dynamics and its Applications to Biological Systems”, 22-15 September 2020.
Title of the seminar: Studying molecular dynamics with an eye to drug design.

Invited speaker at the event AIRC-CAMPUS, University of Naples, 4-5 December 2019, Naples, Italy
Title of the seminar: From computation to drugs.

Invited speaker at the Conference “Computational Advances in Drug Discovery”, Sestri Levante, 23-26 September 2019.
Title of the seminar: Targeting the folding of oncogenic proteins by predicting their local unfolding status.

Invited speaker at the event AIRC-CAMPUS, University of Naples, 20-21 May 2019, Naples, Italy
Title of the seminar: How to discover anticancer drugs.

Keynote speaker at the Conference “Biophysics@Rome”, Rome, Italy, 15-16 May 2019
Title of the seminar: The dynamics of molecular design.

Invited speaker at the Seminar Cycle of the Mario Negri Institute, Milano, Italy 21 March 2019
Title of the seminar: Using Molecular Dynamics in Drug Design.

Invited speaker at the “IDEA of a Centre – Scuola Normale Superiore and Università di Pavia” meeting, Pavia, Italy, 6-7 September 2019
Title of the seminar: The dynamics of molecular design.

Invited speaker at the Cecam Workshop “Protein-peptide interactions: peptide identification, binding prediction and design”, Paris, France, 16-19 October 2018
Title of the seminar: Binding epitope discovery and design.

Invited plenary speaker at the “Convegno 2018 della Divisione di Chimica dei Sistemi Biologici, Società Chimica Italiana”, Caserta, Italy, 26-28 September 2018
Title of the seminar: Combining computational and bioorganic chemistry for the design of new chemical tools

Invited speaker at the KeyLab International Workshop on "Recent computational and experimental advances in molecular medicine", Ho Chi Minh City, Vietnam, 27-29 June 2018
Title of the seminar: Combining computational and bioorganic chemistry for the design of new chemical tools.

Invited speaker at the Cecam Workshop “CompAllo: Towards a Unified Approach to the Analysis and Design of Allostery”, Lausanne, Switzerland, 9-11 April 2018.
Title of the seminar: Controlling molecular chaperones through designed modulators.

Invited speaker at the “Learning from each other” meeting, Kohn Kaen, Thailand, 11-13 February 2018
Title of the seminar: PPI predictions and epitope design: what can computational biology tell us?

Invited seminar at the IRB Institute, Bellinzona, Switzerland, 8 February 2018
Title of the seminar: Protein dynamics and molecular design: computational approaches with an eye to chemical biology

Invited seminar at the Computational Biomedicine Institute Forschungszentrum Jülich, Julich, Germany, 23 January 2018
Title of the seminar: Combining computational and bioorganic chemistry for the design of new chemical tools.

Invited speaker at the Congress “Italy-Japan Joint Symposium - New Trends in Enzyme and Microbial Science in the Translational Biology Era”, Naples, Italy, 18-20 October 2017
Title of the seminar: Protein Protein interactions: Predictions and Design

Speaker at the Congress “Computational Advances in Drug Discovery”, Lausanne, Switzerland, 5-8 September 2017.
Title of the seminar: Protein Protein interactions: Predictions and Design

Distinguished Safra Center Speaker, Tel Aviv University, Tel Aviv, Israel, 16 May 2017
Title of the seminar: Structure-function-dynamics relationships in proteins: implications for drug discovery.

Speaker at the Congress “Molecular Chaperones in Cancer”, Madrid, Spain, 2-4 May 2017
Title of the seminar: Computational studies of the Hsp90 system to design new anticancer molecules.

Invited seminar at University of Aveiro, Aveiro, Portugal, 27 April 2017.
Title of the seminar: Studying protein dynamics to investigate protein-protein interactions.

Invited seminar at Universidad Pompeu Fabra, Barcelona Biomedical Research Park, Barcelona, Spain, 20 January 2017.
Title of the seminar: Computational studies of proteins with an eye to chemical biology.

Speaker at the 8th International Conference on the Hsp90 Chaperone Machine, Seeon, Germany, 2-6 November 2016
Title of the seminar: Computational studies of the Hsp90 system with an eye to drug design.

Invited speaker at the Protein Interactions workshop, Lyngby, Denmark, 26 October 2016.
Title of the seminar: Studying protein dynamics to investigate protein-protein interactions.

Invited speaker at the Sissa Mini-Workshop 2016 on Statistical and Molecular Biophysics, Trieste, Italy, 19-20 October 2016
Title of the seminar: Antigen and epitope design: what can computational biology tell us?

Invited speaker at the FISV 2016, 14th FISV Congress, Rome, Italy, 20-23 September 2016.
Title of the seminar: Antigen and epitope design: what can computational biology tell us?

Speaker at the 251st ACS National Meeting & Exposition, San Diego, California USA, March 13th-17 th, 2016.
Title of the seminar: Dynamics-based drug design: The discovery and development of protein functional activators.

Keynote speaker at the congress “Bologna Peptides 2016”, University of Bologna, Bologna, Italy, February 14th-16th, 2016

Title of the seminar: Protein dynamics and molecular design: computational approaches with an eye to chemical biology.

Invited speaker at the workshop "Computational Molecular Medicine: A mini-symposium dedicated to Ruth Nussinov", University of Aachen, Aachen, Germany, October 21st-23rd, 2015
Title of the seminar: Protein allostery and interactions: computational studies with an eye to chemical biology

Invited speaker at the workshop "Statistical and Molecular Biophysics", SISSA-ISAS Trieste, Italy, October 12-13th, 2015
Title of the seminar: Modifying Protein Functions with Computational and Synthetic Chemistry.

Invited speaker at the conference "SBDD-2015, Computational advances in drug discovery", Lausanne, Switzerland, September 21st-25th, 2015.
Title of the seminar: Modifying Hsp90 Dynamics and Functional Relationships Through Rationally Designed Allosteric Activators

Invited speaker at the European School of Medicinal Chemistry, Urbino, Italy, June 29th-July3rd 2015.
Title of the seminar: Computational Biology in the Design of Allosteric Chemical Chaperones

Speaker at the **Gordon Research Conference**-Bioorganic Chemistry 2015, Andover, NH-USA, June 7th-12th 2015.
Title of the seminar: Modifying Hsp90 Dynamics and Functional Relationships Through Rationally Designed Allosteric Activators

Invited speaker at the workshop "Horizon Chem 2015", Università di Milano Bicocca, Milano, Italy, March 6th 2015
Title of the seminar: Simulazioni molecolari per la progettazione di molecole biologicamente attive con possibili applicazioni terapeutiche e diagnostiche

Invited speaker at the PhD School "Frontiers in Structural Biology", Milano, Italy, November 24th-25th 2014.
Title of the seminar: Computational approaches to molecular design.

Invited speaker at the CECAM-workshop "Advanced modeling to investigate biomolecules", Genova, Italy, November 20th-21st 2014.
Title of the seminar: Rational Design of Modulators of Protein Activities.

Invited speaker at the 7th International Conference on the Hsp90 Chaperone Machine, Seeon, Germany, October 15th-19th 2014.
Title of the seminar: Studying Hsp90 Dynamics with an Eye to Molecular Design.

Invited Keynote speaker at the National Congress of the Italian Chemical Society, Rende, Italy, September 7th-13th 2014.
Title of the seminar: Studying Protein Dynamics with an Eye to Molecular Design.

Invited speaker at the **Gordon Research Conference**-Biopolymers 2014, Newport, RI-USA.
Title of the seminar: Studying Protein Dynamics with an Eye to Molecular Design.

Invited speaker at the PROTSTAB-2014 Meeting, Stresa, Italy, May 7th-9th 2014
Title of the seminar: Studying the determinants of protein stability with an eye to molecular design.

Invited speaker at the ICCMSE-2014 Congress, Athens, Greece, April 4th-7th 2014.
Title of the Seminar: Exploiting conformational dynamics in drug discovery: design of C-terminal inhibitors of Hsp90 with improved activities.

Invited seminar at the University of Milano, Department of Biosciences, Milano, Italy, April 9th 2013.
Title of the Seminar: Computational biology studies of protein dynamics with an eye to drug design.

Invited seminar at the San Raffaele/Dibit series of seminars on Biology and Biophysics. Milano, March 27th 2013.
Title of the Seminar: Molecular simulations of proteins: what are they good for?

Invited speaker at the "CIU 2012 Conference: from genomics to vaccine development research", Khon Kaen, Thailand, October 25-27th 2012.
Title of the Seminar: From antigen structure to epitope prediction and design: a computational biology view

Invited speaker at the "Proteine 2012", Chieti, Italy, September 24-26 2012.
Title of the Seminar: MD simulations of biomolecular machines with an eye to drug design

Invited speaker at the WE-Heraeus Seminar on "Single Molecule Kinetics", Bad Honnef, Germany, July 29-August 1 2012.
Title of the Seminar: Corresponding functional dynamics across the Hsp90 family: insights from a multiscale analysis of MD simulations

Selected speaker at the 2012 ISQBP President's Meeting "Challenges in biomolecular modeling - from QM to coarse-graining". Stockholm, Sweden, June 17-20 2012.
Title of the seminar: MD simulations of biomolecular machines with an eye to drug design

Invited speaker at the CECAM workshop "Anchoring Simulations to Experiments: Challenges for Understanding and Treating Alzheimer's Disease". Paris, France, May 21-23 2012.
Title of the seminar: Identification of Interference Targets and Markers of Protein Aggregation via Molecular Simulations

Invited speaker and chairman of the "Peptides in Drug Design Session" at the PEP-CON Conference,

Beijing, China, March 23-25 2012.
Title of the seminar: Structure-Function-Dynamics Relationships in Proteins: Implications for Drug Design.

Invited seminar at the German Research School for Simulation Sciences (FZ-Juelich), Juelich, Germany, January 31-01-2012.
Title of the seminar: Studying protein dynamics with an eye to drug discovery.

Invited speaker at the CECAM workshop: Innovative Approaches to Computational Drug Discovery, Lausanne, Switzerland, October 3rd-6th 2011.
Title of the seminar: Structure-function-dynamics relationships in proteins: implications for drug discovery

Invited speaker at the SISSA workshop on Structural bioinformatics/biophysics, SISSA, Trieste, Italy, July 7-8th 2011.
Title of the seminar: Investigating protein dynamics with an eye to drug discovery

Invited seminar at SISSA, Trieste, Italy, February 14th 2011.
Title of the seminar: Structure-function-dynamics relationships in proteins: implications for drug discovery

Invited seminar at CEMM, Vienna, Austria, January 12th 2011. Host Giulio Superti-Furga.
Title of the seminar: Investigating protein functions and interactions through computational biology

Invited Plenary Lecture at the Portuguese "National Meeting of Medicinal Chemistry, of the Portuguese Chemical Society", Coimbra, Portugal November 28th-30th, 2010.
Title of the Seminar: Structure-function-dynamics relationships in proteins: implications for drug discovery

Invited speaker at the National Day for Cancer Research organized by AIRC in Salerno, Italy. November 6th, 2010

Invited seminar at the Institute of Protein Biochemistry – CNR, Naples, Italy, November 5th 2010.
Title of the Seminar: Structure-function-dynamics relationships in proteins: implications for drug discovery

Selected speaker at the 2010 meeting "The Hsp90 Chaperone Machine". Les Diablerets, Switzerland, September 29th-October 3rd 2010.
Title of the talk: First *in silico* discovery of allosteric inhibitors of molecular chaperones: Selection of new ligands for the C-terminal Domain of Hsp90

Invited speaker at the 2010 President's Meeting of the ISQBP "Folding and Recognition: Similarities and Differences", Cetraro, Italy, June 14th-16th 2010.
Title of the Talk: In silico discovery of allosteric inhibitors of molecular chaperones: Selection of new

ligands for the C-terminal Domain of Hsp90

Invited speaker at the ESF Workshop "Protist 2010", Istanbul, Turkey, April 23-25th 2010.
Title of the Talk: Investigating protein function and interactions through molecular simulations

Invited seminar at SISSA, Trieste, Italy, April 16th 2010.
Title of the Seminar: Understanding the Function of Biomolecular Machines: What Can Computational Biology Tell Us?

Invited at the Workshop "From Molecular to continuum descriptions of complex materials: dream or reality?" Polytechnic School of Milano, Italy, February 24th 2010.
Title of the Talk: Investigating Protein Stabilization and Interaction Sites through Molecular Simulations.

Invited Seminar at the P2P series of Seminars, University of Padua, Italy, February 19th 2010.
Title of the Presentation: Understanding the Function of Biomolecular Machines: What Can Computational Biology Tell Us?

Invited Talk at the Workshop "Physics of Protein Folding and Aggregation" Brixen, Italy, February 11-12, 2010.
Title of the Talk: Blocking Folding Through Chaperone Inhibition: Signal Propagation Mechanisms and Ligand-Based Conformational Dynamics for the design of New Inhibitors of the Hsp90 Molecular Chaperon

Invited Seminar at the Technical University Munich, Germany, January 26th 2010.
Title of the Presentation: From Molecular Mechanisms to Drug Design: What Can Molecular Simulations Tell Us?

Invited Seminar at the Mount Sinai School of Medicine, New York, NY, USA, June 12th 2009.
Title of the Presentation: Modelling Signal Propagation Mechanisms and Ligand-Based Conformational Dynamics of the Hsp90 Molecular Chaperone Full Length Dimer.

Selected Presentation at the Keystone Symposium "Protein Allostery, Dynamics and Function", Keystone, Colorado USA, June 5-10th 2009.
Title of the Talk: Modelling Signal Propagation Mechanisms and Ligand-Based Conformational Dynamics of the Hsp90 Molecular Chaperone Full Length Dimer.

Invited Seminar at the Department of Biotechnology, Bicocca University, Milano, March 5th 2009
Title of the presentation: From drug design to dynamics and functions of macromolecular machines: What can simulations tell us?

Invited Speaker at the CECAM meeting "Frontiers in aggregation", UCD, Dublin (Ireland), April 29th-May2nd 2009
Title of the Presentation: Investigating and inhibiting peptide aggregation: what can simulations tell us?

Invited Seminar at the ICBP, Paris (France), February 12th 2009.
Title of the Presentation: From molecular recognition to dynamics and functions of macromolecular machines.

Invited Presentation at the Padova University, Padua (Italy), October 20th 2008.
Title of the Presentation: Understanding ligand-based modulation of the Hsp90 molecular chaperone dynamics at atomic resolution.

Invited Seminar at the Max Planck Institute for Biophysical Chemistry, Goettingen (Germany), October 7th 2008.
Title of the Presentation: Investigating and inhibiting peptide aggregation: what can simulations tell us?

Selected Presentation at the ISQBP 2008 President's Meeting, Ascona (Switzerland), June 8th-13th 2008.
Title of the Presentation: Understanding ligand-based modulation of the Hsp90 molecular chaperone dynamics at atomic resolution

Invited Seminar at the Jacobs University Bremen, Bremen (Germany), May 21th 2008.
Title of the Presentation: Molecular Recognition and Drug Design: What Can Simulations Tell Us?

Invited Seminar at the ETH Zurich, host Prof. Michele Parrinello, April 22nd 2008.
Title of the Presentation: Molecular recognition and drug design with MD simulations.

Invited Seminar at the Universitè de Montreal, Montreal (Canada), September 27th 2007.
Title of the Presentation: Molecular Recognition in Biological Systems: What can simulations tell us?

Invited Seminar at McGill University, Montreal (Canada), September 26th 2007.
Title of the Presentation: Molecular Recognition in Biological Systems: What can simulations tell us?

Invited opening lecture at the Congress: "Biophys07; Biology and Beyond" of the National Institute for Nuclear Physics. Arcidosso (Italy), 3-5th September 2007.
Title of the Presentation: Molecular Recognition in Biological Systems: What Can Simulations Tell Us?

Selected Presentation at the Buergenstock Congress on Stereochemistry. Buergenstock (Switzerland), 14-20 April 2007.
Title of the Presentation: Imprint of sequence and structure on the recognition properties of biological systems: insights from molecular simulations.

Invited Seminar at the King's College. London (UK), March 23rd 2007.
Title of the Presentation: Molecular Recognition in Biological Systems: What can simulations tell us?

Invited Seminar at the National Institute for Medical Research. London (UK), March 22nd 2007.
Title of the Presentation: Molecular Recognition in Biological Systems: What can simulations tell us?

Invited Seminar at Nerviano Molecular Science. Nerviano (Italy), July 18th 2006.

Title of the Presentation: Rational Identification of Hsp90 Inhibitors.

Invited Speaker at the International School of Physics "Enrico Fermi": *Protein Folding and Drug Design.* Varenna (Italy), July 4th-July 14th 2006.
Title of the Lecture: Blocking the Protein Folding Machinery, Rational Design of a New AntiCancer Molecule.

Invited Speaker at the International Workshop: *Structural Characterization of Proteins by NMR, X-Ray Crystallography and Computational Methods.* San Vito di Cadore (Italy), June 16th – June18th 2006.
Title of the Plenary Lecture: Simulating Recognition in Biomolecular Systems.

Invited Speaker at the International Workshop: *Protein Aggregation.* CECAM, Lyon (France), May 22nd – May 25th 2006.
Title of the Presentation: Investigating peptide aggregation through MD simulations.

Invited Lecture at the University of Milan, Department of Biology and Biotechnology, January 20th, 2006
Title of the Presentation: Rational Design of inhibitors of the molecular chaperone Hsp90

Invited Speaker at the meeting: *Modelling and Simulation of Biological Systems.*
University of Heidelberg (Germany), November 21st-22nd, 2005-12-2005
Title of the Presentation: Exploring protein folding and misfolding with molecular simulations

Invited Speaker at the *Second P2P Symposium: Predicting the structure and Function of Proteins.* University of Padova, November 10-11th 2005.
Title of the Presentation: The determinants of peptide aggregation: a molecular dynamics view

Invited Speaker at the *1st European Congress on Chemistry for Life Sciences.* October 4-8th 2005.
Title of the Presentation: The determinants of peptide aggregation: a molecular dynamics view

Invited Speaker at the *School of Medicine, University of Massachussets,* April 14th 2005, University of Massachusetts, Worcester, USA.
Title of the Lecture: Exploring protein folding and mis-folding with molecular simulations.

Invited Speaker at the *Department of Physiology and Biophysics, The Mount Sinai School of Medicine,* April 8th 2005, Mount Sinai School of Medicine, New York, USA.
Title of the Lecture: MD simulations in the study of protein folding and drug design.

Award Lecture at the National Congress of the Division of Biological Systems-Italian Chemical Society. November 11th-13th 2004, Caserta, Italy.

Invited Speaker at the Workshop *Theoretical Physics Methods in Quantitative Biology,*
Sept. 23rd-25th 2004, Università di Milano Bicocca, Milano, Italy.
Title of the Presentation: All-atom folding simulations of small protein from stochastically selected coarse grained structures.

Invited Speaker at the *2004 ISQBP President's Meeting, the biannual meeting of the International Society for Quantum Biology and Pharmacology,* June 5-8th 2004, Como, Italy.
Title of the presentation: Study of the Villin Headpiece folding by computing
coarse-grained Monte Carlo evolution and all-atom Molecular dynamics

Invited Lecture at the Department of Organic Chemistry, CSIC Madrid, Spain, April 15-18th 2004.
Title of the Lecture: Molecular Simulations of Biological Systems.

Invited Seminar at Istituto Nazionale per lo Studio e la Cura dei Tumori, Milano January 21st 2004.
Title of the presentation: Mechanism, folding and design of biological systems: what can molecular simulations tell us?

Invited Plenary lecture at the V meeting of the Italian Computational Chemistry Group, December 18-19th 2003, Siena, Italy.
Title of the presentation: QM/MM studies of enzyme selectivity.

Invited lecture at the Faculty of Pharmacy of the University of Coimbra, Portugal, December 4th 2003.
Title of the lecture: Folding, Stability and Mechanisms of Biomolecules. Lessons from Biomolecular simulations.

Invited Speaker at the XXI National Congress of the Italian Chemical Society, June 22-27th 2003, Turin Italy.
Title of the presentation: Folding and Stability of small proteins and peptides: what can MD simulations tell us?

Invited Lecture at the SCMBB-Bruxelles, Universitè Libre Bruxelles (Belgium), May 19th 2003.
Title of the presentation: New Methods to investigate protein folding.

Invited for an Oral Communication at the 2nd *Workshop on Molecular theories and simulations*. Gaeta, Italy, May 13-15th, 2003.
Title of the presentation: Combining Simplified and all-atom methods to investigate protein folding.

Invited Speaker in the Monthly Seminars Series at The department of Chemistry of Penn State University. The Pennsylvania State University, October 11th 2002.
Title of the presentation: The factors influencing the folding and stability of secondary structure forming peptides: MD investigations

Invited for a seminar at the "Abdus Salam international centre for theoretical physics", May 30th 2002, Trieste, Italy.
Title of the presentation: Molecular dynamics simulations of the folding and stability of peptides.

Invited for an Oral Communication at the 1st *Workshop on Molecular theories and simulations*. Gaeta, Italy, May 10-12th, 2002.

Title of the presentation: Simulation MscL gating under pressure.

Invited speaker at the *10th European Congress on Biotechnology* July 8-11th 2001, Madrid, Spain.
Title of the presentation: Understanding Enzyme Mechanism, Stability and Activity via Molecular Simulations

Invited for an Oral Communication at the International Workshop: *Structural characterization of Proteins by NMR, X-ray diffraction and computational methods*. San Vito di Cadore, Italy, September 27-30th, 2001.
Title of the presentation: Folding and Stability of a three stranded β-sheet peptide: Molecular dynamics simulations.

Invited for an Oral Communication at the International Congress: *Biostabilization.* Lisbon, Portugal April 9-12th, 2000.
Title of the Presentation: Stability and Activity of a Mesophilic Protein and its Thermophilic Homolog: Insights from Molecular Dynamics Simulations.

Invited for a seminar at the "Instituto de Quimica Organica General (CSIC)", July 11th 2001 Madrid, Spain.
Title of the presentation: Molecular dynamics simulations of three stranded β-peptides folding

Invited for an Oral Communication at the "*Giornata di studio della divisione dei sistemi biologici della Società Chimica Italiana – Modeling and computational methods: New perspectives in the study of folding and binding mechanisms of biomolecules*" March 29th 2001, Milano, Italy
Title of the presentation: Molecular dynamics simulations of three stranded β-peptides folding

Invited for an Oral Communication at the *10th Annual Biomos Meeting* September 6-8th 2000, Burg Arras, Alf-Mosel, Germany.
Title of the presentation: Folding and Stability of the Three-Stranded-β peptide Betanova: Insights from Molecular Dynamics Simulations

Invited for an Oral Communication at the International Symposium: *Modulation of enzyme properties by protein and medium engineering.* October 20th, 2000, Milano, Italy.
Title of the Presentation: Stability and Activity of a Mesophilic Protein and its Thermophilic Homolog: Insights from Molecular Dynamics Simulations.