Curriculum Vitae et Studiorum
for GIORGIO COLOMBO

PERSONAL DATA

Full Name: Giorgio Colombo

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

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 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

Appointed as contract professor for the "Bioinformatics" course at the faculty of Biotechnology, University of Milano, year 2004.
Appointed as contract professor for the course "Molecular Simulations of Biochemical Systems", SISSA-ISAS Trieste, year 2011-2012.
Appointed as contract professor for the course "Molecular Simulations of Biochemical Systems", SISSA-ISAS Trieste, year 2012-2013.
Appointed as contract professor for the course "Molecular Simulations of Biochemical Systems", SISSA-ISAS Trieste, year 2013-2014.
Professor for the masters course "Drug Design and Development", Faculty of Pharmacy, University of Coimbra, year 2013-2014.

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 Sistems 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 XXXVII edition of the "Attilio Corbella" Summer School on Organic Synthesis. Gargnano (BS), Italy, June 18-22 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 Master - 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 Master - Università Statale di Milano.

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

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

Supervisor of PhD Theses and Thesis Committees.

- 2003-2004. Protein folding and protein stability: a molecular dynamics perspective. Candidate Giacomo M.S. De Mori, PhD school in Chemical Sciences - Università Statale di Milano.

- 2004-2005. Biomolecular simulations by classical dynamics. Candidate Stefano Pieraccini, PhD school in Chemical Sciences - Università Statale di Milano.

- 2005-2006. Molecular dynamics simulations of molecular recognition in biological processes. Candidate Massimiliano Meli, PhD school in Chemical Sciences - Università Statale di Milano.

- 2007-2008. Supervisor of the thesys 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.

- 2009-2010. 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.

- Since 2011-2012, Supervisor of the PhD thesis work of Claudio Peri, PhD School in Biological and Molecular Sciences - Università Statale di Milano.

- ICREA (Spain)
- AICR (Scotland)
- ANR (France)
- KNOW (The Netherlands)

INDUSTRIAL COLLABORATIONS

2002-2004	Scientific Consultant for "Vicuron S.P.A." in the field of drug design of new antibiotic molecules. (60 K€)
2002-2003	Scientific Consultant for "Nicox Research Institute S.r.l.". (15 K€)
2007	Scientific Consultant for "EOS, Ethical Oncology Science, Milano" (20 K€)
Since September 2009	Scientific Consultant for "Kemotech S.r.l".

MEMBERSHIPS AND DUTIES FOR SCIENTIFIC SOCIETIES

June 2010-2014	Elected Councilor of the International Society for Quantum Biology and Pharmacology (ISQBP)
Since 2005	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 (95-98), MS-DOS Set up and run a HPC cluster
Programming Languages:	C, Fortran
Known Programs:	Biochemical Systems Simulation: AMBER, ROAR,DivCon, MACROMODEL, Biosym-Insight, GROmacs

- Since 2011-2012, Supervisor of the PhD thesis work of Maria Armandina Cruz de Jesus Baptista, Faculdade de Farmacia, Universidade de Coimbra (Portugal).

- 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. 2008.

- 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.

- 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.

REFEREE ASSISTANCE FOR JOURNALS and FUNDING BODIES

Dr. Colombo is a Member of the Editorial Board of
- *PLoS ONE*
- *BMC Structural Biology.*

Reviewer Duties for Scientific Journals
- Nature Chemical Biology
- 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

Reviewer Duties for Funding Agencies and Scientific Societies
- Israel Science Foundation
- Reviewer for the 7th Framework Programme of the European Community

Gaussian94, Midas Plus
Utility Programs
Microsoft Word, Excel, Isis-Draw Microsoft Office.

MAIN GRANTS

- **Title of the project:** Thrombospondin-1 domains affecting angiogenesis and tumour behaviour.
  Funding Organization: Italian Association for Cancer Research (AIRC).
  Duration: 2004-2007
  Role in the project: Head of operating unit, Co-PI
  Funding received: 60000€

- **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€

- **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€

- **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€

- **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€

- **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€

- **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€

- **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€

- **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€

- **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€

- 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.

- **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)

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€

- **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€

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

MOST RELEVANT INVITATIONS AND PRESENTATIONS

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.
Titol 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.

POSTER Communications to Congresses

EMBL-EBI/Wellcome Trust course: Resources for Computational Drug Discover; Hinxton, Cambridge, UK 2-6 July 2012
Peri, C.; Morra, G.; Scarabelli, G.; **Colombo, G.**
Analyzing dynamic and energetic preorganization to study protein interactions

2012 Italian Bioinformatics Society Annual Meeting – BITS2012, Catania (Italy) May 2-4, 2012
Corrada, D.; Morra, G.; **Colombo, G.**

A Structure Based Pattern Recognition on Antibodies" -

2010 SCI Congress San Vito di Cadore, Italy
Genoni, A.; Morra, G.; Merz, K.M. Jr.; **Colombo, G.**
Unraveling the resistance shown by the Subtype B / HIV Protease to currently known inhibitors by means of computational studies

2010 SCI Congress San Vito di Cadore, Italy
Torella, R.; Moroni, E; Caselle, M.; Morra, G.; **Colombo, G.**
Dynamic and Energetic Determinants of Protein-DNA recognition

2010 SCI Congress San Vito di Cadore, Italy
Scarabelli, G.; Morra, G.; **Colombo, G.**
Predicting interaction sites from the energetics of isolated proteins: a new approach to epitope mapping

50th Sanibel Symposium, St. Simons Island (Georgia, USA), February 24 - March 2, 2010
Genoni, A.; Morra, G.; Merz, K.M. Jr.; **Colombo, G.**
Dynamic and energetic explanation of the HIV-1 protease drug resistance

Thermodinamically Unstable Proteins: Chance or Necessity?" Trieste (Italy), December 14-16, 2009
Genoni, A.; Morra, G.; Merz, K.M. Jr.; **Colombo, G.**
Computational study of the resistance shown by the Subtype B / HIV-1 protease to currently known inhibitors.

2009 SCI Congress Sorrento, Italy
G. Scarabelli, G. Morra, **G. Colombo**
Ab initio epitope prediction based on the dynamics and energetics of protein antigens

2009 The European Protein Society meeting. June 14th-18th, Zurich, Switzerland.
Poster Titled: Modeling signal propagation mechanisms and ligand based conformational dynamics of the Hsp90 molecular chaperone

2009 Keystone Symposium on Protein Dynamics, Allostery and Function. June 5th-10th, Keystone, CO, USA.
Poster Titled: Modeling signal propagation mechanisms and ligand based conformational dynamics of the Hsp90 molecular chaperone

2008 The 4th International Conference on the Hsp90 Chaperone Machine. October 2nd-6th 2008, Seeon, Bavaria Germany.
Poster Titled: Ligands modulate the functional motion of Hsp90 by driving the residue-residue interdomain communication: a molecular dynamics study.
Poster Titled: Understanding ligand based modulation of the Hsp90 molecular chaperone dynamics at atomic resolution.

2007 European Protein Society Meeting, May 12-16th 2007, Stockholm, Sweden
Poster Titled: Computational Studies of the Structure, Dynamics and Native Content of Amyloid-like Fibrils of Ribonuclease A.

2006 ISQBP President's Meeting, the biannual meeting of the International Society for Quantum Biology and Pharmacology, June 24-27th 2004, Strasbourg, France
Poster Titled: Rational Identification of a New Anti-Cancer Compound.

2005 First European Conference on Chemistry for Life Sciences. October 4-8th 2005, Rimini, Italy.
Poster Titled: Rational Design of Sheperdin, a Novel Anticancer Agent.

2004 Gordon Research Conference on Biopolymers, June 13-18th 2004, Newport RI, USA.
Poster Titled: All-atom folding simulations of Small Proteins from stochastically-selected coarse-grained structures

2004 ISQBP President's Meeting, the biannual meeting of the International Society for Quantum Biology and Pharmacology, June 5-8th 2004, Como, Italy
Poster Titled: All-atom folding simulations of Small Proteins from stochastically-selected coarse-grained structures

SCI Workshop: "From Genes to Molecules", February 8-10th, 2002. Certosa di Pontignano, Siena, Italy.
1 Poster Titled: Molecular dynamics simulations of secondary structure forming peptides in 2,2,2-trifluoroethanol/water mixtures. (Winner of the best poster award) M. Fioroni, D. Roccatano and **G. Colombo.**
2 Poster Titled: Reverse turn mimetic bicyclic lactams: Application to the design of beta-hairpin like peptides. L. Belvisi, **G. Colombo,** M. Colombo, L. Manzoni, D. Potenza, C. Scolastico.

ESS Workshop: "Flexibility and Function of Proteins", January 25-27th, 2002. Heidelberg, Germany.
Poster Titled: A systematic molecular dynamics study of the conformational behavior of Betanova and its mutants. P. Soto, **G. Colombo,** A.E. Mark

Workshop on Carbohydrate Recognition, September 21th, 2001 Università di Milano, Milano Italy.
Poster Titled: Design and synthesis of ganglioside GM1 mimics. D. Arosio, A. Bernardi, G. Colombo, S. Sonnino, D. Potenza.

FEBS Forum of Young Scientists. Protein Structure-Function, Trafficking and Signaling. Instituto de Tecnologia Quimica e Biologica ITQB, June 28-30th, 2001. Oeiras, Portugal.
Poster Titled: A molecular dynamics study of a three stranded antiparallel beta-sheet forming peptide and some of its mutants. P.Soto, **G. Colombo,** A.E. Mark

27th meeting of the Federation of European biochemical societies FEBS. June 30th to July 5th 2001, Lisbon, Portugal
Poster Titled: A molecular dynamics study of a three stranded antiparallel beta-sheet orming peptide

and some of its mutants. P.Soto, **G. Colombo**, A.E. Mark

Conference of the SIMU Programme "Bridging the Time-Scale Gap", Konstanz, Germany, September 10 -13, 2001.
Poster Titled: A molecular dynamics study of a three stranded antiparallel beta-sheet forming peptide and some of its mutants. P.Soto, **G. Colombo**, A.E. Mark

Biotrans 1999. 4th International conference on Biocatalysis and Biotransformations. Taormina, Italy. September 26-October 1 1999.
1 Poster Titled: Rationalization of the enantioselectivity of subtilisin in DMF and hexane. **G Colombo**, G. Ottolina, G. Carrea, K.M. Merz, Jr.
2 Poster Titled: Enzymatic modification of natural glycosides: the case of stevioside and steviolbioside. **G. Colombo**, B. Danieli, S. Riva.

ACADEMIC REFERENCES:

Prof. Kenneth M. Merz, Jr.
PO Box 118435
Gainesville, FL 32611, USA
Office: 2328 New Physics Building
Phone: ++1-352-392-6973
E-mail: merz@qtp.ufl.edu

Prof. Alan E. Mark
Molecular Dynamics Group
School of Chemistry and Molecular Biosciences (SCMB)
University of Queensland
Brisbane, QLD 4072,
Australia
Physical address:
Rm 331 Level 3, Molecular Biosciences Building (#76)
Email: a.e.mark@uq.edu.au
Secretary: md.secretary@uq.edu.au
Phone: +61-7-3365 4180
FAX: +61-7-3365 3872
Secr: +61-7-3365 3821

Prof. Arjan Van der Vaart
University of South Florida
Department of Chemistry
4202 E. Fowler Ave. CHE 205
Tampa, FL 33620
Tel.: 813-974-8762
Fax.: 813-974-3203
Email: vandervaart@cas.usf.edu

Dr. Franca Fraternali
Randall Division of Cell and Molecular Biophysics
New Hunt's House (room 3.14)
King's College London, Guy's Campus
SE1 1UL London UK
E-mail: franca.fraternali@kcl.ac.uk
tel (direct) +44-(0)-207-8486843
fax +44-(0)-207-8486435

Prof. Roman Osman
Department of Physiology and Biophysics
One Gustave L. Levy Place, Box 1218
New York, NY 10029, USA
E-mail: roman.osman@mssm.edu

Dr. Giulia Taraboletti
Head of the Tumor Angiogenesis Unit
Department of Oncology
Mario Negri Institute for Pharmacological Research
Bergamo, Italy
Tel: ++39-035-319888
E-mail: taraboletti@marionegri.it

Prof. Dario C. Altieri
Director, The Wistar Institute Cancer Center
Executive Vice President
Chief Scientific Officer
Robert and Penny Fox Distinguished Professor
Phone: ++1-215-495-6975, Office
E-mail: daltieri@Wistar.org

Gio Colombo