MARCO DE VIVO

Curriculum Vitae

Istituto Italiano di Tecnologia (IIT)
Laboratory of Molecular Modeling and Drug Discovery
Drug Discovery and Development Department
Via Morego 30, Genoa I-16163, Italy

Contents

CURRENT POSITION

09/2013 – Present	**Research Lab Director, *Tenured Senior Researcher***
Institute	**Molecular Modeling and Drug Discovery Lab** **Istituto Italiano di Tecnologia (IIT)**

Reseach activities: My group investigates the structure, dynamics, and catalysis of chemical systems. Our goal is to understand the general principles that control molecular recognition and catalysis, and to use this information to design intelligent nanosystems and potent inhibitors for drug discovery. The group fully integrates computational and synthetic chemistry with molecular and structural biology for computational enzyme design, catalysis and drug discovery.

05/2009 – 08/2013	**Team Leader in Computational Chemistry** **Project Leader in Drug Discovery**
Institute	**Istituto Italiano di Tecnologia (IIT)**

Research activities: During this period, D3-IIT was organized as an integrated matrix organization, with project leaders of drug discovery programs. In addition to supervising one PhD student and one postdoc in computational chemistry, I was Project Leader of two multidisciplinary teams for drug discovery. Each team comprised 5-10 scientists, including team leaders, postdocs, and PhD students in computational and medicinal chemistry, advanced NMR fragment-based screening, X-ray crystallography, bioanalytical chemistry, and pharmacology.

PROFESSIONAL EXPERIENCE

09/2015 – 12/2017	**Research Associate (affiliation while in IIT)**
Institution	**Forschungszentrum Jülich, Germany**
Research	IAS-5 / INM-9 Computational Biomedicine

03/2007 – 05/2009	**Research Scientist - Project leader and computational chemist for structure-based drug design and discovery**
Institution	**Rib-X Pharmaceuticals, Inc. (New Haven, CT – USA)**
Supervisor	Dr. Erin M. Duffy – CSO at Rib-X (now Melinta Therapeutics)

Role: Leadership and computational support of a multidisciplinary team focused on drug discovery of novel antibiotics. The team used structure-based drug design to target the ribosome in order to treat antibiotic-resistant infections.

Contribution: Discovering novel compounds with antibacterial activity, coordinating the discovery effort, and working in close collaboration with crystallographers, biochemists, medicinal chemists, and pharmacologists (see Patents & Inventions).

03/2004 – 03/2007	**Postdoctoral Researcher**
	Prof. Michael L. Klein's group **University of Pennsylvania (UPenn), Philadelphia PA – USA** **Center for Molecular Modeling, Dept. of Chemistry**
Research	Enzymatic catalysis and ligand binding in metalloproteins
01/2003 – 05/2003	**Visiting Scientist**
	Swiss Federal Institute of Technology (ETH in Zürich – Switzerland) **Institute of Pharmaceutical Sciences**
Supervisor	Prof. Leonardo Scapozza
Research	Virtual screening of small molecules to inhibit protein kinases
08/2001 – 12/2002 **06/2003 – 12/2003**	**Visiting Scientist**
	International School for Advanced Studies (SISSA) in Trieste, Italy
Supervisor	Prof. Paolo Carloni
Research	QM, Car-Parrinello QM/MM and classical MD simulations of protein kinase CDK2

EDUCATION

01/2001 – 02/2004
PhD student in Pharmaceutical Sciences
University of Bologna, Italy, Dept. of Pharmaceutical Sciences

Subject of Thesis	Computational Methods in Medicinal Chemistry
Thesis	*Computational Study of Cyclin-Dependent Kinases (CDKs): Reaction Mechanism and Conformational Flexibility*
Advisors	Prof. Paolo Carloni, Prof. Andrea Cavalli
Supervisor	Prof. Maurizio Recanatini

07/1999 – 09/2000
Undergraduate student
2000 BA and MSc in Chemistry (Italian Laurea)
University of Bologna, Italy, Dept. of Chemistry

Subject of Thesis	Computational Organic Chemistry
Thesis	Computational Investigations of Enzymatic Reactions: Lysozyme and HIV- Integrase
Advisor	Prof. Fernando Bernardi
Supervisor	Prof. Andrea Bottoni

AWARDS, HONORS AND RECOGNITIONS

2020 Director of the CECAM Node CECAM-IT-SIMUL (https://cecamsul.eu)

2019 Associate Editor of Journal of Chemical Theory and Computation *(ACS Publications)*

2019 Advisory Board Member of Chem *(Cell Press)*

2019 Advisory Board Member of Journal of Chemical Information and Modeling *(ACS Publications)*

2019 International Meetings Liaison, ACS COMP division**.**

2018 Habilitation as Full Professor in Medicinal Chemistry, in Italy.

2018 Member of the Scientific Committee for Associazione Italiana per la Ricerca sul Cancro **(AIRC) -** The Italian Association for Cancer Research

2017 Scientific Advisory Board Member of BiKi Technologies, an IIT spin-off that develops software for computer-aided drug discovery

2017 ACS COMP Division - Outstanding Junior Faculty Award, ACS

2014 Habilitation as Associate Professor in Medicinal Chemistry, in Italy.

2013 My First AIRC Grant (MFAG); talented Italian < 40 years old, for cancer research

2006 O1 Visa – Issued by the United States Immigration Office for demonstrated extraordinary ability in the field of science.

2003 Marco Polo Fellowship for excellent research projects funded by Uni. Bologna.

TEACHING EXPERIENCE

I teach structure-based drug design (SBDD) and molecular modelling to PhD students at IIT for 4-6 hours every year, since 2009. I have delivered a number of invited lectures on drug discovery and SBDD (see below) at institutions in Italy and abroad.

Before joining IIT, my teaching experience included:

2006 - Teacher during the Quantum Chemistry II course (Spring Course, CHEM 524) for Graduate Students, University of Pennsylvania, Philadelphia (6-hour lesson).

2002, 2003 - Laboratory Assistant for the Advanced Methods in Medicinal Chemistry course, held by Dr. Andrea Cavalli at the Dept. of Pharmaceutical Sciences, Uni. Bologna.

LAB MEMBERS, SUPERVISED STUDENTS AND POSTDOCS

CURRENT MEMBERS

Researchers

Sept 2019 – present | **Dr. Pietro Vidossich** - Researcher (comp chem)

May 2013 – present | **Dr. Laura Riccardi** - Research Associate (comp chem) since 2019
Postdoc between 2013 - 2018

Postdocs

21 July 2021 – present I **Rigoldi Federica** (comp chem)
Affiliated from University of Padova AIRC IG Grant 2020 N. 25003

1 January 2021 – present I **Ilaria Silvestri** (biochem) AIRC IG GRANT 2019 N. 23679

1 Nov 2020 – present I **Marco Borgogno** – (med chem) AIRC IG GRANT 2019 N. 23679

1 April – present | **Andrea Menichetti** – (med chem) AIRC IG GRANT 2019 N. 23679

1 March 2020 – present | **Ankita Sarkar** – (comp chem) AIRC - iCARE 2 Fellowship N. 23979

15 February 2020 – present | **Isabella Acquistapace** (bio chem) AIRC IG GRANT 2019 N. 23679

1 October 2019 – present | **Amos Funagalli** (biochem, shared 50% with Cancedda's Lab)

1 Feb 2019 – present | **Inacrist Geronimo** – (comp chem)

Feb 2018 – present | **Nicoletta Brindani** – (med chem)

Graduate Fellows

Nov 2020 – present | **Alessandro Andreani** – PhD Student (med chem)

Oct 2019 – present | **Manuel Jose Ruiz Munevar** – PhD Student (comp chem)

Oct 2019 – present | **Maria Antonietta La Serra** – PhD Student (comp chem)

Oct 2019 – present | **Michela Nigro** – PhD Student (bio chem)

Nov 2017 – present | **Sebastián Franco Ulloa** – PhD Student (comp chem) AIRG IG grant 18883
I served as Advisor for his undergrad Thesis performed in my Lab at IIT in 2014/2015

Sep 2017 – present | **Jacopo Manigrasso** – PhD Student (comp chem)

Jul 2017 – present | **Elisa Donati** – PhD Student (comp chem)

Nov 2018 – present | **Federico Munafò** – PhD Student (med chem)

Jan 2020 – present | **Bharath Raghavan** – PhD Student (comp chem) shared with Prof. Carloni's Lab through IIT – Julich FZ Agreement, funded by The Helmholtz Association

PAST MEMBERS

PhD students

Nov 2016 – Oct 2019 | **Marco Borgogno** – Graduated April 2020
I served as Supervisor for his PhD at IIT

Nov 2014 – Nov 2017 I **Elirosa Minniti** – Graduated April 2018
I served as Supervisor for her PhD at IIT

Sep 2013 – Dec 2017 I **Vito Genna** – Graduated April 2017
I served as Supervisor for his PhD at IIT. He obtained a postdoc position with Prof. M. Orozco at IRB Barcelona and he received an EMBO Fellowship.

Jan 2014 – Apr 2017 I **Giuseppina La Sala** – Graduated Apr 2017
I served as Supervisor for her PhD at IIT. She obtained a position at BiKi Technologies as an Application Scientist, now at AstraZeneca.

Jan 2010 – Sept 2013 I **Giulia Palermo** – Graduated April 2013
I served as Supervisor for her PhD at IIT. She first obtained a postdoc position at EPFL with Prof. Rothlisberger, then postdoc with Prof. A. McCammon and now Assistant Prof. at UC Riverside in USA.

2009 – 2012 I **Sai Vikrama Chaitanya Vummaleti** – Graduated April 2012
I served as Advisor for his PhD at IIT.

Postdocs

1 Jun 2019 – 31.06.2021I **Dr. Corinne Portioli** – (biochem, shared 50% with Cancedda's Lab)

1 Jan 2018 – 31.05.2021 | **Dr. Adam Pecina** – (comp chem)

Adam received the 'Seal of Excellence' – Marie Curie (IF) fellowship in 2018

Adam received a Marie Curie (IF) fellowship in my Lab starting in June 2019

Jun 2014 – 31 Oct 2019 | **Dr. Jose M. Arencibia** – (biochem)
Jose is on external budget (AIRG IG grant 18883)

1 Nov 2017 – 31 Oct 2019 | **Dr. Jissy Kuriappan** – (comp Chem)
Jissy is recipient of a Marie Curie (IF) fellowship in my Lab, starting November 2017

Sep 2013 – January 2018 | **Dr. Jose Antonio Ortega Martínez** – postdoc (med chem)
Jose became Researcher in Dr. Cavalli's Lab, at IIT.

Oct 2012 – Dec 2013 | **Dr. Marino Convertino** – (comp chem)**,** postdoc under my supervision at the IIT-D3, Genoa. Marino became a postdoc at Uni. North Carolina with Prof. Dokholyan

Master students

Oct 2018 – 31 Oct 2019 | **Matteo Borella** – Graduate Student (comp chem)
I served as co-supervisor for his undergrad Thesis performed in my Lab at IIT in 2018/2019

Jan 2016 – Apr 2016 | **Sebastián Franco Ulloa** - undergraduate (comp chem)
Visiting from Universidad de los Andes (Colombia).
I served as Co-Advisor for his undergraduate thesis, defended in Colombia in May 2016.

SCIENTIFIC ACTIVITIES

2021 **Co-Chair**, Panel for the Portuguese public funding agency (FCT), R&D funds.

2020 **Committee Member** for the dissertation of PhD candidate Andrés Felipe Vásquez Jiménez at Universidad de Los Andes. Supervisor: Prof. Andrés Fernando Gonzalez Barrios.

2020 **Committee Member** for the dissertation of PhD candidate Von Erlach Thibaud at the EPFL, Lausanne – Dept. of Chemistry. Supervisor: Prof. Ursula Rothlisberger.

2019 **IIT Representative** at Board of the CECAM Node IT-SIMUL

2018 **Grant Reviewer** PRIN (Progetti di Rilevante Interesse Nazionale), Italy.

2018 **Depositor of 2 pdb structures:** Protein Tyrosine Phosphatase 1B A122S mutant (PDB ID: 6CWV) and Protein Tyrosine Phosphatase 1B F135Y mutant (6CWU)

2018 **Committee Member** for the PhD dissertation for the 30° cycle of the PhD course in chemical, geological and environmental chemistry at the University of Milano Bicocca.

2017 **Judge** for the Excellence Award for Graduate Students applications for the 2018 Spring national ACS meeting (New Orleans, LA)

2017 **Grant Reviewer** for the Chemical Theory, Models and Computational Methods program in the Chemistry Division of U.S. NSF (National Science Foundation) - Early Faculty Career Development Program (CAREER)

2017 **Member of the Scientific Advisory Board** of the 22nd EuroQSAR Symposium, which will be held in Thessaloniki, Greece, between 16-20 September, 2018.

2017 **Committee Member** (Collegio dei Docenti) for the Data Science and Computation PhD at University of Bologna.

2017 **Grant Reviewer** for a Veni grant within the Innovational Research Incentives Scheme, Netherland.

2016 **Chairman** at the CECAM workshop (23-25 May) in Pisa, IT-SNS entitled Structural and Functional Annotation of Bioinorganic Systems: Perspectives and Challenges from Theory and Experiments

2016 **Contributor** to the Human Technopole (HT) Masterplan https://multimedia.iit.it/asset-bank/assetfile/6907.pdf (HT is a new research Institute in Milan, Italy).

2016 **Thesis Co-advisor** for the Chemistry bachelor thesis of Sebastian Franco Ulloa, Uni. de los Andes (CO).

2015 **IIT Representative** at the CECAM Council meeting in Lausanne (19-20 Nov)

2015 **Local Organizing Committee Member** of the 21st EuroQSAR Symposium, held 4-8 September 2016 in Verona (IT).

2015 **Committee Member** for the PhD dissertation of Hassan Pezeshgi Modarres at the EPFL, Lausanne – School of Life Sciences, Institute of Bioengineering. Supervisor: Prof. Matteo Dal Peraro.

2015 **Grant Reviewer** for the National Research, Development and Innovation Office (NKFIH), the main organization in Hungary for channeling funds to (basic) research.

2015 Grant Reviewer for the SIR Programme (Scientific Independence of Young Researchers) in Italy

2014 **Committee Member** for the dissertation of PhD candidate Polydefkis Diamantis at the EPFL, Lausanne – Dept. of Chemistry. Supervisor: Prof. Ursula Rothlisberger.

2014 **Grant Reviewer** for the Czech Science Foundation
2013, 2014 2015, 2016, 2017: **Committee Member** (Collegio dei Docenti) for the PhD in Pharmaceutical and Biological Sciences at Uni. Bologna

2013 **Committee Member** for the dissertation of PhD candidate Xiaojing Cong at the International School for Advanced Studies (SISSA) in Trieste, Italy. Supervisors: Prof. Paolo Carloni, and Prof. Giuseppe Legname.

2013 **Grant Reviewer** for Marie Curie COFUND for the EU 7th Framework Programme .

2013 **Grant Reviewer** for the Italian Projects of Relevant National Interest(PRIN).

2013 **Grant Reviewer** for LinkSCEEM/Cy-Tera HPC (multi-Tflops facility in Cyprus) – Computer time allocation.

2013 **Panel Member** for the 6th Regular Project Access call of PRACE (Partnership for Advanced Computing in Europe) in Brussels.

2012 **Committee Member** for the exam for master students at EPFL, Lausanne. School of Life Sciences, Institute of Bioengineering. Candidate: Pandey Gaurav. Supervisor: Prof. Matteo Dal Peraro.

2012 **Committee Member** for the 1st year PhD exam at EPFL, Lausanne. School of Life Sciences, Institute of Bioengineering. Candidate: Hassan Pezeshgi Modarres. Supervisor: Prof. Matteo Dal Peraro.

2011 **Session Chairman** during the Computationally driven drug discovery meeting, held 21-23 November at the Auditorium of Research Center of Dompé SpA, L'Aquila (IT)

2011 **IIT-D3 Representative** in the task force to create a large compound library for the Italian Drug Discovery Network (IDDN)

2011 – Present **Peer Reviewer** for PRACE

2011 – Present **Peer Reviewer** for ISCRA (Italian SuperComputing Resource Allocation - CINECA)

2010: **Panel Member** for the 1st Regular Project Access call from PRACE.

2009 **Peer Reviewer** for the IIT Seed Funds.

2009 **Committee Member** for the 1st year PhD exam at EPFL, Lausanne. School of Life Sciences, Institute of Bioengineering. Candidate: Matteo Thomas Degiacomi. Supervisor: Prof. Matteo Dal Peraro

2008, 2009 **Poster Committee Member** for the International Society for Computational Biology + European Conference on Computational Biology conference.

2008 **Judge** for The Emerging Technologies Competition Symposium at the 236th American Chemical Society National Meeting, Philadelphia.

2005, 2006 **Grant Reviewer** for The Kentucky Science and Engineering Foundation.

2004-2007 **Contributing Proposal Writer** for computational resources at the Pittsburgh Supercomputing Center and the National Center for Supercomputing Applications.

Peer Reviewer for:

Nature; Nature Chemical Biology; Nature Reviews Chemistry; Nature Communications; Proceedings of the National Academy of Sciences - USA; Journal of the American Chemical Society; Chem (Cell Press); ACS Catalysis; Journal of Chemical Theory and Computation; Journal of Medicinal Chemistry; ACS Chemical Neuroscience; ACS Medicinal Chemistry Letters; ACS Chemical Biology; Structure; Chemical Communication; Journal of Chemical Information and Modeling; Journal of Physical Chemistry B; Plos Computational Biology; Plos One; Proteins: Structure, Function, and Bioinformatics; Journal of Computer-Aided Molecular Design; Journal of Molecular Modeling; European Journal of Medicinal Chemistry; Bioorganic & Medicinal Chemistry Letters; Chemical Biology & Drug Design; Chemical Physics Letters; Current Pharmaceutical Design; BMC Structural Biology; Bioinformatics; Physical Chemistry Chemical Physics; FEBS Journal; Journal of Enzyme Inhibition and Medicinal Chemistry; Chemistry Central Journal; Journal of the American Association of Pharmaceutical Scientists; Biomolecules; Inorganica Chimica Acta; Biochimica et Biophysica Acta - General Subjects Frontiers Chemistry etc…

ORGANIZATION OF SCIENTIFIC EVENTS

Proposer and Co-organizer

2022 INTERNATIONAL CONFERENCE
Computational Advances in Drug Discovery

TBC, Italy, September 2022

2020 INTERNATIONAL CECAM WORKSHOP
Frontiers of Quantum and Classical Modeling of Metals in Biological Systems
CECAM-FR-IDF, Paris (FR), 8-10 July à Postponed to 2022

2019 INTERNATIONAL CONFERENCE
Computational Advances in Drug Discovery
Sestri Levante, Italy (IT) on 23-26 September

2019 INTERNATIONAL CECAM WORKSHOP
Progress and developments of artificial intelligence for drug design
Genova, at IIT, Italy 17-19 June (IT)

2019 INTERNATIONAL CECAM WORKSHOP
Challenges in modeling and simulations of nanoparticles in complex environments
Genova, at IIT, Italy 29-31 May (IT)

2018 INTERNATIONAL CECAM WORKSHOP
Frontiers and challenges of computing metals for biochemical, medical and technological applications
CECAM-FR-IDF, Paris (FR), 11- 13 July

2017 INTERNATIONAL CONFERENCE
Computational Advances in Drug Discovery
SwissTech Convention Center@EPFL, Lausanne (CH) on 5-8 September

2015 INTERNATIONAL CECAM WORKSHOP
Modeling activity vs. selectivity in metalloproteins
CECAM-FR-IDF, Paris (FR), 29 June - 1 July

2015 INTERNATIONAL CECAM CONFERENCE
Computational Advances in Drug Discovery conference of the year
SwissTech Convention Center@EPFL, Lausanne (CH), 22-25 September

2014 INTERNATIONAL CECAM WORKSHOP
Advanced modeling to investigate biomolecules
D3 Dept. at IIT, Genoa (IT), 20-21 November

2013 INTERNATIONAL CECAM WORKSHOP
Second Innovative Approaches to Computational Drug Discovery workshop
CECAM-HQ, Lausanne (CH), 1-4 October

2011 INTERNATIONAL CECAM WORKSHOP
First Innovative Approaches to Computational Drug Discovery workshop
CECAM-HQ, Lausanne (CH), 3-5 October

Co-organizer

2015 INTERNATIONAL MINISYMPOSIUM
International minisymposium in honor of Prof. R. Nussinov
Jülich Research Center, Jülich (DE) on 22 October

2006 WORKSHOP
First Users Meet Developers workshop on QM/MM simulations
Center for Molecular Modeling, Philadelphia (US), 28-30 September

GRANTS

To date, I have secured **~2.5 Milion Euros** (2014-present) through competitive extramural grants. In addition, I have received **tens of millions of computing core hours** with several peer-reviewed funded grants for computational time on European Supercomputers (High Performance Computing), including **3 major PRACE grants**.

ONGOING GRANTS

	01/01/2020 – 31/12/2024
Agency	**Associazione Italiana per la Ricerca sul Cancro (AIRC)** **T*he Italian Association for Cancer Research***
	Grant Investigator Grant (23769) – 2019
Project title	Development of novel small molecules that inhibit the growth of early stage melanoma tumors
PI	Marco De Vivo
FUNDS	**951,000 Euros**

	01/01/2020 – 31/12/2022
Agency	**Helmholtz Society (Helmholtz European Partnering call)**
Project title	Innovative high-performance computing approaches for molecular neuromedicine
Co-PI at FZJ in Germany	Paolo Carloni, Giulia Rossetti, Bernd Neumair
Co-PI at IIT	Marco De Vivo**,** Laura Cancedda, Michele Parrinello
FUNDS	**1Milion Euros shared in personnel**

PAST GRANTS

	01/06/2019 – 31/05/2021
Agency	**European Commission, MSCA-IF-2017 - Individual Fellowships**
Project title	Metal-dependent catalysis of nanozymes: First steps towards computational nanoenzymology
PI (Host)	Marco De Vivo - Applicant: Adam Pecina
FUNDS	**183, 473 Euros**

	01/06/2019 – 31/05/2021
Agency	**European Commission, MSCA-IF-2017 - Individual Fellowships**
Project title	Structural and functional insights into NKCC1 devoid of diuretic effects
Co-PI (Host)	Marco De Vivo and Laura Cancedda **-** Applicant: Corinne Portioli
FUNDS	**168,369.60 Euros** (shared 50% with Cancedda's Lab)

	01/01/2016 – 01/01/2021
Agency	**Telethon - (Dulbecco telethon carrier award program) Italy**
Project title	Targeting aberrant Cl- homeostasis and GABAA transmission to design innovative therapeutic approaches in Down syndrome.
PI	Laura Cancedda, IIT (Granted 600,000 euros)
My Role	Collaborator (AT NO COST)
	01/06/2019 – 30/05/2020
	Agency ISCRA (Italian Super Computing Resource Allocation) - Class C Projects
Project title	A molecular dynamics-based strategy for allosteric pocket detection
PI	Marco De Vivo
Granted	40,000 core-h on MARCON2 @ CINECA
	01/01/2017 – 31/12/2019
Agency	**Associazione Italiana per la Ricerca sul Cancro (AIRC) -** The Italian Association for Cancer Research
Grant	Investigator Grant (18883) - 2016
Project title	Design and characterization of RhoJ Interaction Inhibitors as a Novel Therapy for Stage III Melanoma
PI	Marco De Vivo
FUNDS	**308,000 Euros**
	01/11/2017 – 31/10/2019
Agency	**European Commission, MSCA-IF-2016 - Individual Fellowships**
Project title	Mechanistic studies of metal-dependent DNA cleavage in Type II topoisomerase toward the rational design of novel anticancer drugs
PI (Host)	Marco De Vivo **-** Applicant: Jissy Kuriappan
FUNDS	**180,070 Euros**
	03/04/2018 – 12/04/2019
Agency	**PRACE** (Partnership for advanced computing in Europe)
Project title	NANOMOTION - Monolayer protected gold nanoparticles, on the move: Toward the design of nanoparticles with programmed recognition abilities
PI	Marco De Vivo
Granted	**36,000,000 core-h on Marconi-KNL (Cineca, Italy) – Tier-0 project** Approximately equivalent to 250,000 Euros
	01/01/2017 – 31/12/2017
Agency	**ISCRA** (Italian SuperComputing Resource Allocation) - Class B Projects
Project title	Enzymatic processing and selectivity of lipids Deciphering lid-domain function and plasticity in lipases
PI	Marco De Vivo
Granted	**4,000,000 core-h on MARCON2 @ CINECA** Approximately equivalent to 30,000 Euros

	02/01/2014 – 31/03/2017
Agency	**Associazione Italiana per la Ricerca sul Cancro (AIRC)**
	The Italian Association for Cancer Research
Grant	**My First AIRC Grant – MFAG (14140) - 2013**
Project title	Acid ceramidase inhibition as a novel strategy to treat malignant melanoma
PI	Marco De Vivo
FUNDS	**210,000 Euros**

	04/03/2014 – 03/03/2015
Agency	**PRACE** (Partnership for advanced computing in Europe)
Project title	Lipid degradation in the endocannabinoid system: Deciphering specificity in FAAH catalysis
PI	Marco De Vivo
Granted	**13,900,000 core-h on CURIE FN (GENCI@CEA, France) – Tier-0 project**
	Approximately equivalent to 750,000 Euros

	01/11/2012 – 31/10/2013
Agency	**PRACE** (Partnership for advanced computing in Europe)
Project title	Enhanced sampling simulations to investigate the binding of potent anticancer drugs to the human Type II topoisomerase
PI	Marco De Vivo
Granted	**5,000,000 core-h on CURIE FN (GENCI@CEA, FR) – Tier-0 project**
	Approximately equivalent to 250,000 Euros

	01/01/2011 – 31/12/2011
Agency	**ISCRA** (Italian SuperComputing Resource Allocation) - Class A Projects
Project title:	Enhanced sampling simulations to investigate the catalytic metal binding site of Type II topoisomerases
PI	Marco De Vivo
Granted	**1,000,000 core-h on IBM-SP6 @ CINECA**
	Approximately equivalent to 50,000 Euros

	01/11/2015 – 31/10/2016
Agency	**John von Neumann Institute for Computing** (NIC) - Germany
Project title	Mechanism and Energetics of the nucleotidyl-transfer reaction catalyzed by DNA Polymerase-eta
PI	Dr. Emiliano Ippoliti (German Research School for Simulation Sciences)
Granted	**550,000 core-h on JURECA at the Jülich Supercomputing Centre**
Collaborators	Marco De Vivo and Vito Genna (PhD Student in De Vivo's group)
	Approximately equivalent to 100,000 Euros

	01/11/2014 – 31/10/2015
Agency	**John von Neumann Institute for Computing** (NIC) - Germany
Project title	Mechanism and Energetics of the nucleotidyl-transfer reaction catalyzed by DNA polymerase-eta

PI	Dr. Emiliano Ippoliti (German Research School for Simulation Sciences)
Granted	**300,000 core-h on JUROPA at the Jülich Supercomputing Centre**
Collaborators	Marco De Vivo and Vito Genna (PhD Student in De Vivo's group)
	Approximately equivalent to 55,000 Euros

PATENTS AND INVENTIONS

Inventions at IIT:

12. **IT 102019000004929**
    Patent filed on new compounds targeting Intracellular chloride concentration
    Modulators Of Intracellular Chloride Concentration
    Cancedda L., De Vivo M., Contestabile A., Borgogno M., Savardi A., Ortega Martinez J. A.

11. **EP18170092.3**
    Patent filed on new compounds targeting the prion protein
    Serpin inhibitors for the treatment of prion and prion-like diseases
    Legname G., Vanni S., Carloni P., De Vivo M.

10. **IT 102017000047189**
    Patent filed on new compounds targeting the protein RhoJ
    Compounds and composition for the treatment of cancer, retinal disorders, and cardiomyopathies
    De Vivo M., Ganesan A., Ortega Martinez J. A., Jahid S.

9. **IT 102017000028709**
    Patent filed on new anticancer compounds targeting topoisomerases
    5-carboxamide-2-thiobarbituric acids and use thereof as medicaments
    De Vivo M., Ortega Martinez J. A., Arencibia Jimenez J. M., Sissi C.

8. **IT 102017000012144**
    Patent filed on new anticancer compounds targeting the acid ceramidase enzyme
    Acid Ceramidase inhibitors, and their use as medicaments
    De Vivo M., Ortega Martinez J.O.

7. **IT 102016000130706 (UA2016A009452)**
    Patent filed on new anticancer compounds targeting topoisomerases
    4-amino-2-pyrido-bicyclic pyrimidines as type II topoisomerase inhibitors and use thereof as medicaments
    De Vivo M., Ortega Martinez J. A., Arencibia Jimenez J. M., Minarini A., Sissi C.

6. **PCT/EP2015/060291**
    Benzoxazolone derivatives as acid ceramidase inhibitors, and their use as medicaments
    Piomelli D., Pagliuca C., Pizzirani D., Bach A., Realini N., De Vivo M.

5. **PCT/EP2012/065336 (Granted in EP, US, JP, IT, DE, FR, GB, AUS)**
    Multitarget FAAH and COX inhibitors and therapeutical uses thereof
    De Vivo M., Scarpelli R., Cavalli A., Migliore M., Piomelli D., Habrant D., Favia A.D.

4. **PCT/EP2012/061662**
    Carprofen derivatives as inhibitors of FAAH and/or COXs
    De Vivo M., Scarpelli R., Cavalli A., Favia A.D., Habrant D., Piomelli D.

Inventions outside IIT

Joint inventor of 3 inventions at Rib-X Pharmaceuticals (now Melinta Therapeutics):

Antimicrobial compounds and methods of making and using the same

These three international applications have entered national stages in **tens** of nations/regions worldwide, with **nine patents already granted**:

3. **PCT/US2010/052928**
   Duffy E., Bhattacharjee A., O'Dowd H., De Vivo M., Du Y., Sinishtaj S., Tang Y., Wimberly B.
2. **PCT/US2010/052924**
   Duffy E., Bhattacharjee A., O'Dowd H., Chen S., De Vivo M., Lou R., Wimberly B.
1. **PCT/US2010/052922**
   Duffy E., Bhattacharjee A., O'Dowd H., De Vivo M., Kanyo Z., Martinow J., Paik I., Scheideman M., Sinishtaj S., Wimberly B., Wu Y.

PUBLICATIONS

(h-index 32, ~3003 citations – Google Scholar - July 28, 2021)

ARTICLES – REVIEWS - BOOKS

(* indicates when I am the only or joint corresponding author)

85. J. Manigrasso, M. Marcia, M. De Vivo*
Computer-aided design of RNA-targeted small molecules: a growing need in drug discovery
Chem (Cell Press), 2021 - Available online

84. J. Manigrasso, M. De Vivo*, G. Palermo
Controlled Trafficking of Multiple and Diverse Cations Prompts Nucleic Acid Hydrolysis
ACS Catal., 2021 - Available online
Cover Article

83. M. Marcia, J. Manigrasso, M. De Vivo,*
Finding the ion in the RNA-stack: Can computational models accurately predict key functional elements in large macromolecular complexes?
J. Chem. Inf. Model. 2021 - Available online

82. A. Pecina, D. Rosa-Gastaldo, L. Riccardi, S. Franco-Ulloa, E. Milan, P. Scrimin, F. Mancin, M. De Vivo*
On the Metal-Aided Catalytic Mechanism for Phosphodiester Bond Cleavage Performed by Nanozymes
ACS Catal. 2021, 11, 14, 8736–8748 Link
Cover Article

81. M. Borgogno, A. Savardi, J. Manigrasso, A. Turci, C. Portioli, G. Ottonello, S. M. Bertozzi, A. Armirotti, A. Contestabile, L. Cancedda, M. De Vivo*
Design, synthesis, in vitro and in vivo characterization of selective NKCC1 inhibitors for the treatment of core symptoms in Down syndrome and other brain disorders
J. Med. Chem. 2021 - Available online
Cover Article

80. L. Riccardi, S. Decherchi, W. Rocchia, G. Zanoni, A. Cavalli, F. Mancin, M. De Vivo*
Molecular recognition by gold nanoparticle-based receptors as defined through surface morphology and pockets fingerprint
J. Phys. Chem. Lett., 2021, 12, 23, 5616–5622 Link
Cover Article

79. C. Portioli, M. J. Ruiz Munevar, M. De Vivo*, L. Cancedda
Cation-coupled chloride cotransporters: chemical insights and disease implications
Trends in Chemistry (Cele Press), 2021 - In Press

78. S. Franco-Ulloa, D. Guarnieri, L. Riccardi, P. Pompa and M. De Vivo*
Association mechanism of peptide-coated metal nanoparticles with model membranes: A coarse-grained study
J. Chem. Theory Comput., 2021 - In Press

77. P. Vidossich and M. De Vivo*
The role of first principles simulations in studying (Bio)catalytic processes
Chem Catalysis (Cell Press), 2021 - In Press

76. L. Morillas-Becerril, S. Franco-Ulloa, I. Fortunati, R. Marotta, X. Sun, G. Zanoni, M. De Vivo*, F. Mancin
Arginine magic with gold nanoparticles: specific and nondisruptive interaction with neutral phospholipid bilayers
Communications Chemistry (Nature), 2021 - In Press

75. I. Geronimo, P. Vidossich, E. Donati, M. De Vivo*
Computational investigations of polymerase enzymes: Structure, function, inhibition, and biotechnology
WIREs Computational Molecular Science, **2021 - In Press**

74. M. Prejanò, P. Vidossich, N. Russo, M. De Vivo*, T. Marino
Insights into the catalytic mechanism of domains CD1 and CD2 in Histone Deacetylase 6 from quantum calculations
ACS Catal., 2021 - In Press

73. P. Vidossich, M. Castañeda, E. Luis, C. Mota, D. de Sanctis, G. P. Miscione, M. De Vivo*
Functional Implications of Second-shell Basic Residues for dUTPase DR2231 Enzymatic Specificity
ACS Catal., 2020 - 10, 23, 13825–13833

72. J. A. Ortega, J. Arencibia, E. Minniti, J.O. Byl, S. Franco-Ulloa, M. Borgogno, V. Genna, M. Summa, S. M. Bertozzi, R. Bertorelli, A. Armirotti, A. Minarini, C. Sissi, N. Osheroff, M. De Vivo*
A novel, potent, and drug-like tetrahydroquinazoline inhibitor that is highly selective for human topoisomerase II α over β
J. Med. Chem. 2020, 21, 12873–12886

71. S. Franco-Ulloa , G. Tatulli , S. Løland Bore , M. Moglianetti , P. P. Pompa ,M. Cascella, M. De Vivo*
Dispersion state phase diagram of citrate-coated metallic nanoparticles in saline solutions
Nat. Comm., 2020, 11, 5422

70. J. Czescik, S. Zamolo, T. Darbre, C. Sissi, A. Pecina, L. Riccardi, M. De Vivo*, F. Mancin, P. Scrimin
A Gold Nanoparticle Nanonuclease Relying on a Zn(II) Mononuclear Complex
Angewandte Chemie, 2020, 59, 2 – 12

69. Savardi, M Borgogno, R. Narducci, G. La Sala, J. Ortega, M. Summa, A. Armirotti, R. Bertorelli, A. Contestabile, M. De Vivo*, L Cancedda
Discovery of a small molecule drug candidate for selective NKCC1 inhibition in brain disorders
Chem (Cell Press) 2020, 6, 1–24

68. J. Manigrasso, I. Chillón, V. Genna, P. Vidossich, S. Somarowthu, A. M. Pyle, M. De Vivo*, M. Marco
Visualizing Group II Intron Dynamics between the First and Second Steps of Splicing
Nat. Comm., **2020, 11, 2837**

67. E. Catanzaro, N. Betari, J. M. Arencibia, S. Montanari, C. Sissi, A. De Simone, I. Vassura, A. Santini, V. Andrisano, V. Tumiatti, M. De Vivo, D. V. Krysko, M. B.L. Rocchi, C. Fimognari, A. Milelli
Targeting Topoisomerase II with Trypthantrin Derivatives: Discovery of 7-((2-(dimethylamino)ethyl)amino)indolo[2,1-b]quinazoline-6,12-dione as an Antiproliferative Agent to Treat Cancer
Eur. J. Med. Chem. 2020, 202 (15), 112504

66. D. Duarte, A. Lamontanara, G. La Sala, S. Jeong, Y-K Sohn, A. Panjkovich, S. Georgeon, T. Kükenshöner, M. Marcaida, F. Pojer, M. De Vivo, D. Svergun, H-S Kim, M. Dal Peraro, Oliver Hantschel
Btk SH2-kinase interface is critical for allosteric kinase activation and its targeting inhibits B-cell neoplasms
Nat. Comm. 2020*, 11, 2319*

65. J. Arencibia, N; Brindani, S. Franco-Ulloa, M. Nigro,, J. A. Kuriappan, G. Ottonello, S. Mandrup Bertozzi, M. Summa, S. Girotto, R. Bertorelli, A. Armirotti, M. De Vivo*
Design, synthesis, dynamic docking, biochemical characterization, and in vivo pharmacokinetics studies of novel topoisomerase II poisons with promising antiproliferative activity
J. Med. Chem. 2020, **63, 7, 3508-3521**

64. E. Donati, V. Genna, and M. De Vivo*
Recruiting mechanism and functional role of the third metal ion in the enzymatic activity of 5' structure-specific nucleases
J. Am. Chem. Soc., 2020, 142 (6), pp 2823-2834

63. J. A. Kuriappan, N. Osheroff, and M. De Vivo*
Smoothed Potential MD Simulations for Dissociation Kinetics of Etoposide to Unravel IIsoform Specificity in Targeting Human Topoisomerase II
J. Chem. Inf. Model., 2019, 59 (9), pp 4007-4017

62. S. Vanni, L. Riccardi, G. Palermo, and M. De Vivo*
Structure and Dynamics of the Acyl Chains in the Membrane Trafficking and Enzymatic Processing of Lipids
Acc. Chem. Res., 2019, **52 (11), pp 3087 – 3096**

61. V. Genna, M. Marcia, and M. De Vivo*
A Transient and Flexible Cation-Pi Interaction Promotes Hydrolysis of Nucleic Acids in DNA and RNA Nucleases
J. Am. Chem. Soc., 2019, 141 (27), pp 10770-10776

60. L. Riccardi, F. De Biasi, M. De Vivo, T. Burgi, F. Rastrelli, and G. Salassa
The Dynamic Origin of Chirality Transfer between Chiral Surface and Achiral Ligand in Au38 Clusters
ACS Nano, 2019. 58 (23), pp 7702-7707

59. X. Sun, L. Riccardi, F. De Biasi, F. Rastrelli, M. De Vivo,* and F. Mancin
Molecular Dynamics Simulation-Directed Rational Design of Nanoreceptors with Targeted Affinity
Angewandte Chemie, 2019, 58 (23), pp 7702-7707

58. S. Franco-Ulloa, L. Riccardi, F. Rimembrana, M. Pini, M. De Vivo*
NanoModeler: A Webserver for Molecular Simulations and Engineering of Nanoparticles
J. Chem. Theory Comput., 2019, 15 (3), pp 2022–2032
Cover Article

57. V. Genna, E. Donati, M. De Vivo*
The Catalytic Mechanism of DNA and RNA Polymerases (Perspective)
ACS Catalysis, **2018, 8 (12), pp 11103–11118**

56. M. Hjortness, L. Riccardi, A. Hongdusit, P. Zwart, B. Sankaran, M. De Vivo, J. M. Fox
Evolutionary Conserved Allosteric Communication in Protein Tyrosine Phosphatases
Biochemistry, **2018**, **57 (45), pp 6443–6451**

55. M. Hjortness, L. Riccardi, A. Hongdusit, A. Ruppe, M. Zhao, E. Kim, P. Zwart, B. Sankaran, H. Arthanari, M. Sousa, M. De Vivo, J. M. Fox
Abietane-Type Diterpenoids Inhibit Protein Tyrosine Phosphatases by Stabilizing an Inactive Enzyme Conformation
Biochemistry, **2018, 57 (40), pp 5886–5896**

54. L. Riccardi, V. Genna, M. De Vivo*
Metal-ligand interactions in drug design (Perspective)
Nature Reviews Chemistry, **2018, 2, 100–112**

53. A. A Oviatt, J. A Kuriappan, E. Minniti, K. R. Vann, P. Onuorah, A. Minarini, M. De Vivo*, N. Osheroff

Polyamine-containing etoposide derivatives as poisons of human type II topoisomerases: Differential effects on topoisomerase IIa and IIb
Bioorg. Med. Chem. Lett., **2018**, **28, 2961-2968**

52. V. Genna, P. Carloni, M. De Vivo*

A strategically located Arg/Lys residue promotes correct base paring during nucleic acid biosynthesis in polymerases
J. Am. Chem. Soc., 2018, 140 (9), pp 3312–3321
Cover Article

51. S. Franco-Ulloa, G. La Sala, G.P. Miscione, M. De Vivo*

Novel Bacterial Topoisomerase Inhibitors Exploit Asp83 and the Intrinsic Flexibility of the DNA Gyrase Binding Site
Int. J. Mol. Sci. 2018, 19(2), 453 (Special Issue on Topoisomerase

50. V. Genna, M. Colombo, M. De Vivo*, M. Marcia

Second-shell basic residues expand the two-metal-ion architecture of DNA and RNA processing enzymes
Structure (Cell Press), 2018, 26, 40–50

49. J. A. Ortega, L. Riccardi, E. Minniti, M. Borgogno, J. M. Arencibia, M. L. Greco, A. Minarini, C. Sissi, M. De Vivo*

Pharmacophore hybridization to discover novel Topoisomerase II poisons with promising antiproliferative activity
J. Med. Chem., 2018, **61 (3), pp 1375–1379**
Cover Article

48. E. Minniti, J. A. W. Byl, L. Riccardi, C. Sissi, M. Rosini, M. De Vivo, A. Minarini, N. Osheroff

Novel xanthone-polyamine conjugates as catalytic inhibitors of human topoisomerase II
Bioorg. Med. Chem. Lett., 2017, 27, 4687–4693

47. G. La Sala, S. Decherchi, M. De Vivo*, W. Rocchia

Allosteric communication networks in proteins revealed through pocket crosstalk analysis
ACS Central Science, 2017, 3 (9), pp 949–960
Highlighted in First Reactions *ACS Central Science*, Toward Understanding the Ways of Allosteric Drugs, by R. Amaro **2017**. ***3*** **(9), pp 925–926**
Cover Article

46. J. A. Ortega, J. M. Arencibia, G. La Sala, M. Borgogno, L. Bono, A. Armirotti, S. Girotto, A. Ganesan, **M. De Vivo***

Pharmacophore identification and scaffold exploration to discover novel, potent and chemically stable inhibitors of acid ceramidase in melanoma cells
***J. Med. Chem.,* 2017, *60* (13), pp 5800–5815**

45. **M. De Vivo*** and A. Cavalli
Recent advances in dynamic docking for drug discovery (Opinion)
WIREs Computational Molecular Science, 2017, 7:e1320
Cover Article

44. L. Riccardi, L. Gabrielli, X. Sun, F. De Biasi, F. Rastrelli, F. Mancin, M. De Vivo*
Nanoparticle-based receptors mimic protein-ligand recognition
Chem (Cell Press), **2017**, 3, 92–109
Cover Article for July 2017

43. L. Riccardi, J.M. Arencibia, L. Bono, A. Armirotti, S. Girotto, M. De Vivo*
Lid domain plasticity and lipid flexibility modulate enzyme specificity in human monoacylglycerol lipase
BBA - Molecular and Cell Biology of Lipids, **2017**, **862(5):441-451**

42. M. De Vivo*, M. Masetti, G. Rossetti
BOOK CHAPTERS - **Invited contribution**
"Molecular modelling and simulations applied to challenging drug discovery targets"
in "**Computational Tools for Chemical Biology**", **Royal Society of Chemistry, 2017**
Edited: Sonsoles Martín-Santamaría

41. J. Dreyer, G. Brancato, E. Ippoliti, V. Genna, M. De Vivo, P. Carloni, U. Rothlisberger
BOOK CHAPTERS - **Invited contribution**
"First Principle Methods in Biology: From Continuum Models to Hybrid Ab Initio Quantum Mechanics/Molecular Mechanics"
in "**Simulating Enzyme Reactivity**" - Published by **The Royal Society of Chemistry, 2017**
Edited by Iñaki Tuñón and Vicente Moliner

40. G. La Sala, L. Riccardi, R. Gaspari, A. Cavalli, O. Hantschel, M. De Vivo*
HRD motif as the central hub of the signaling network for activation loop autophosphorylation in Abl kinase
J. Chem. Theory Comput., 2016, 12 (11), pp 5563–5574
Cover Article for 8 November 2016 issue

39. V. Genna, P. Vidossich, E. Ippolito, P. Carloni, M. De Vivo*
A self-activated mechanism for nucleic acid polymerization catalyzed by DNA/RNA polymerases
J. Am. Chem. Soc., **2016**, 138 (44), pp 14592–14598
Highlighted in JACS Spotlights, Polymerases May Progress with the Help of Hydrogen Bonding, by Deirdre Lockwood (Ph.D.)
J. Am. Chem*. Soc.*, **2016, 138 (44), pp 14507–14508**
Cover Article for 9 November 2016 issue

38. M. Pavlin, G. Rossetti, M. De Vivo, P. Carloni

Carnosine and Homocarnosine Degration Mechanisms by the Human Carnosinase Enzyme CN1: Insights from Multiscale Simulations
Biochemistry, 2016 – 55 (19), pp 2772–2784

37. V. Genna, R. Gaspari, M. Dal Peraro, M. De Vivo*

Cooperative motion of a key positively charged residue and metal ions for DNA repair catalyzed by Y-family polymerases
Nucleic Acid Res., **2016, 44 (6): 2827-2836**
Cover Article for 7 April 2016 issue

36. **M. De Vivo***, M. Masetti, G. Bottegoni, A. Cavalli

The role of molecular dynamics and related methods in drug discovery
J. Med. Chem., 2016, 59 (9), pp 4035–4061
Recommended by F1000 Prime (two recommendations)

35. G. Palermo, A.D. Favia, M. Convertino, M. De Vivo*

The Molecular Basis for Dual Fatty Acid Amide Hydrolase (FAAH)/Cyclooxygenase (COX) Inhibition
ChemMedChem, **2016**, **Volume 11, Issue 12, Pages 1252–1258**

34. G. Palermo, E. Minniti, M. L. Greco, L. Riccardi, E. Simoni, M. Convertino, C. Marchetti, M. Rosini, C. Sissi, A. Minarini, M. De Vivo*

An optimized polyamine moiety boosts potency of human type II topoisomerase poisons as quantified by comparative analysis centered on the clinical candidate F14512
Chem. Comm., **2015**, 51, 14310 – 14313
Cover Article (Back cover for October 2015 issue)

33. G. Palermo, I. Bauer, P. Campomares, A. Cavalli, A. Armirotti, S. Girotto, U. Roethlisberger, M. De Vivo*

Keys to lipid selection in FAAH catalysis: Structural flexibility, gating residues and multiple binding pockets
Plos Comp. Biol., **2015, 11(6): e1004231**
Cover Article for June 2015 issue

32. G. Palermo, A. Cavalli, M. L. Klein, M. Alfonso-Prieto, M. Dal Peraro, M. De Vivo*

Catalytic metal ions and enzymatic processing of DNA and RNA
Acc. Chem. Res., **2015 Feb 17;48(2):220-8**

31. D. Pizzirani, A. Bach, N. Realini, A. Armirotti, L. Mengatto, I. Bauer, S. Girotto, C. Pagliuca, M. De Vivo, M. Summa, A. Ribeiro, D. Piomelli

Benzoxazolone-Carboxamides: Potent systemically active inhibitors of intracellular Acid Ceramidase
Angew. Chem. Int. Ed. Engl., **2015 Jan 7;54(2):485-9**

30. G. Palermo, U. Roethlisberger, A. Cavalli, M. De Vivo*
Computational insights into function and inhibition of FAAH
Eur. J. Med. Chem., 2015 Feb 16;91:15-26 (Review)

29. G. Palermo, P. Campomares, A. Cavalli, U. Roethlisberger, M. De Vivo*
Anandamide hydrolysis in FAAH reveals a dual strategy for efficient enzyme-assisted amide bond cleavage via nitrogen inversion
J. Phys. Chem. B, **2015** Jan 22;119(3):789-801
Special Issue, W. L. Jorgensen's 65th birthday

28. G. Palermo, M. De Vivo*
BOOK CHAPTERS - **Invited contribution**
Computational Chemistry for Drug Discovery
Encyclopedia of Nanotechnology, **Springer** – **2015, pp 1-15**

27. M. Cascella, M. Dal Peraro, M. De Vivo*
BOOK CHAPTERS - **Invited contribution**
Computational chemistry strategies tackling function and inhibition of pharmaceutically relevant targets
Pp. 290-343 (54) in Volume 1 of the eBooks series entitled
Frontiers in Computational Chemistry by **Bentham Science Publishers** – **2015**

26. M. De Vivo*
BOOK REVIEW - **Invited contribution**
Enzyme Technologies: Pluripotent Players in Discovering Therapeutic Agents.
Edited by Hsiu-Chiung Yang, Wu-Kuang Yeh, James R. McCarthy (Wiley)
ChemMedChem - Volume 10, Issue 8, page 1443, August 2015

25. G. Palermo, P. Campomares, M. Neri, D. Piomelli, A. Cavalli, U. Roethlisberger, M. De Vivo*
Wagging the tail: essential role of substrate flexibility in FAAH catalysis
J. Chem. Theory Comput., **2013**, 9 (2), pp 1202–1213

24. G. Palermo, M. Stenta, A. Cavalli, M. Dal Peraro, M. De Vivo*
Molecular simulations highlight the role of metals in catalysis and inhibition of type II topoisomerase
J. Chem. Theory Comput., **2013**, **9 (2), pp 857–862 (Letter)**
Cover Article for February 2013, Vol. 9 Num. 2

23. L. Bertolacci, E. Romeo, M. Veronesi, P. Magotti, C. Albani, M. Dionisi, C. Lambruschini, R. Scarpelli, A. Cavalli, M. De Vivo, D. Piomelli, G. Garau
A binding site for non-steroidal anti-inflammatory drugs in Fatty Acid Amide Hydrolase
J. Am. Chem. Soc., 2013 Jan 9;135(1):22-5 (Communication)

22. A.D. Favia, D. Habrant, R. Scarpelli, M. Migliore, C. Albani, S. M. Bertozzi, M. Dionisi, G. Tarozzo, D. Piomelli, A. Cavalli, M. De Vivo*

    Identification and characterization of carprofen as a multitarget fatty acid amide hydrolase/Cyclooxygenase inhibitor
    J. Med. Chem., 2012, 55 (20), pp 8807–8826

21. S. V. C. Vummaleti, D. Branduardi, M. Masetti, M. De Vivo, R. Motterlini, A. Cavalli

    Theoretical Insights into the Mechanism of Carbon Monoxide (CO) Release from CO-Releasing Molecules
    Chemistry: A European Journal, **2012, Vol. 18, Issue 30, 9267-9275**

20. A. Lodola, D. Branduardi, M. De Vivo, L. Capoferri, M. Mor, D. Piomelli, A. Cavalli

    A catalytic mechanism for cysteine N-terminal nucleophile hydrolases, as revealed by free energy simulations
    PLoS One, **2012, 7(2), e32397**

19. A. Lodola and M. De Vivo*
    BOOK CHAPTERS - Invited contribution
    The increasing role of QM/MM in drug discovery
    in "**Structural and mechanistic enzymology: Bringing together experiments and computing**",
    Edited by Christo Z. Christov and Tatyana Karabencheva-Christova, **Elsevier** – **2012**

18. G. Palermo, D. Branduardi, M. Masetti, A. Lodola, M. Mor, D. Piomelli, A. Cavalli, M. De Vivo*

    Covalent inhibitors of fatty acid amide hydrolase: A rationale for the activity of piperidine and piperazine aryl ureas
    J. Med. Chem., 2011, 54 (19), 6612–6623

17. M. De Vivo, G. Bottegoni, A. Berteotti, M. Recanatini, F.L. Gervasio, A. Cavalli

    Cyclin-dependent Kinases: Bridging their Structure and Function through Computations
    Future Med. Chem., **Sep;3(12):1551-9, 2011 (Review)**

16. D. Branduardi, M. De Vivo, N. Rega, V. Barone, A. Cavalli

    Methyl phosphate dianion hydrolysis in solution characterized by path collective variables coupled with DFT-based enhanced sampling simulations
    J. Chem. Theory Comput., **2011**, **7, 539-543 (Letter)**

15. M. De Vivo*

    Bridging Quantum Mechanics and Structure-Based Drug Design
    Front. Biosci., **2011**, **Jan 1; 16: 1619-1633. (Review)**

14. M. H. Ho, M. De Vivo, M. Dal Peraro, M. L. Klein

    Understanding the Effect of Magnesium Ion Concentration on the Catalytic Activity of Ribonuclease H through Computation: Does a Third Metal Binding Site Modulate Endonuclease Activity?

J. Am. Chem. Soc., **2010, 132, 13702-13712.**

13. M. H. Ho, M. De Vivo, M. Dal Peraro, M. L. Klein
Unraveling the Catalytic Pathway of Metalloenzyme Farnesyltransferase through QM/MM Computation
J. Chem. Theory Comput., **2009, 5, 1657-1666.**

12. M. De Vivo*, M. Dal Peraro, M. L. Klein
Phosphodiester Cleavage in Ribonuclease H occurs via an Associative Two-Metal-Aided Catalytic Mechanism
J. Am. Chem. Soc., **2008 130(33),10955-62.**
Highlighted in *JACS Select* 2008, 130 (50),16824–16827.

11. M. De Vivo, A. Cavalli, P. Carloni, M. Recanatini
Computational Study of the Phosphoryl Transfer Catalyzed by a Cyclin-Dependent Kinase
Chemistry: A European Journal, **2007 13(30), 8437-44.**

10. M. De Vivo*, B. Ensing, M. Dal Peraro, G. A. Gomez, D. W. Christianson, M. L. Klein
Proton Shuttles and Phosphatase Activity in Soluble Epoxide Hydrolase
J. Am. Chem. Soc., **2007, 129(2), 387-394.**

9. M. Dal Peraro, K. Spiegel, G. Lamoureux, M. De Vivo, W. F. DeGrado, M. L. Klein
Modeling the Charge Distribution at Metal Sites in Proteins for Molecular Dynamics Simulations
J. Struct. Biol., 2007, **157(3), 444-453.**

8. B. Ensing, M. De Vivo, Z. Liu, P. Moore, M. L. Klein
Metadynamics as a Tool for Exploring Free Energy Landscape of Chemical Reactions
Acc. Chem. Res., **2006, 39, 73.**

7. M. De Vivo, A. Cavalli, G. Bottegoni, P. Carloni, M. Recanatini
Role of Phosphorylated Thr160 for the Activation of the CDK2/Cyclin A Complex
Proteins, 2006, **62, 89-98.**

6. M. De Vivo*, B. Ensing, M. L. Klein
Computational Study of Phosphatase Activity in Soluble Epoxyde Hydrolase: High Efficiency through a Water Bridge Mediated Proton Shuttle
J. Am. Chem. Soc., **2005**, **127(32), 11226-11227. (Communication)**

5. A. Bottoni, G.P. Miscione, M. De Vivo
A Theoretical DFT Investigation of the Lysozyme Mechanism. Computational Evidence for a Covalent Intermediate Pathway
Proteins, **2005, 59, 118-130.**
Recommended by F1000 (by Prof. A. Warshel)

4. A. Cavalli, G. Bottegoni, C. Raco, M. De Vivo, M. Recanatini

   A Computational Study of the Binding of Propidium to the Peripheral Anionic Site of Human Acetylcholinesterase
   J. Med. Chem., **2004**, **47, 3991-3999.**

3. E. G. Occhiato, A. Ferrali, G. Menchi, A. Guarna, G. Danza, A. Comerci, R. Mancina, M. Serio, G. Garotta, A. Cavalli, M. De Vivo, M. Recanatini

   Synthesis, Biological Activity, and Three-Dimensional Quantitative Structure-Activity Relationship Model for a Series of Benzo[c]quinolizin-3-ones, Nonsteroidal Inhibitors of Human Steroid 5alpha-Reductase 1
   J. Med. Chem., **2004, 47, 3546-3560.**

2. A. Cavalli^, M. De Vivo^, M. Recanatini (^Co-first author)

   Density Functional Study of the Enzymatic Reaction Catalyzed by a Cyclin-Dependent Kinase
   Chem. Comm., **2003**, **1308-1309.**

1. F. Bernardi, A. Bottoni, M. De Vivo, M. Garavelli, G. Keserü, G. Náray-Szabó

   A Hypothetical Mechanism for HIV-1 Integrase Catalytic Action: DFT Modeling of a Bio-mimetic Environment
   Chem. Phys. Lett., 2002, 362, 1-7.

INVITED LECTURES AND SEMINARS

2021, June 28 – July 1 – Virtual Edition
European School of Medicinal Chemistry ESMEC40th Advanced Course of Medicinal Chemistry and Seminar for PhD students
Mechanistic insights into bacterial group II intron RNA catalysis

2021, April 29
Pharmacelera, New frontiers in CNS - Session 1: From target selection to small molecules design
Webinar: *Discovery of selective NKCC1 inhibitors for the treatment of brain disorders*

2020, October 1
University Bologna, Dept. Pharmaceutical Chemistry, Rimini (IT)
Computation for Drug Discovery

2020, 21-25 September 26,
ICTP-SISSA-CECAM Workshop on Molecular Dynamics and its Applications to Biological Systems – **Trieste (IT)**

2020, 16 – 21 August – postponed to 2022
WATOC 2020 (USA)

2020, 19 – 24 July, 2020 – postponed to 2022
GRC – Gordon Research Conference (SP)

2020, 28 June – 2 July – postponed to 2021
ESMEC – European School of Medicinal Chemistry (IT)

2020, March 11 – postponed
EPFL School of Life Sciences, Lausanne (CH)
Structure-Based Drug Design, as part of the Biomolecular Structure and Mechanics course for Master students within the Institute of Bioengineering

2020, 29 – 31 March, 2020 - postponed
CECAM - Centre Européen de Calcul Atomique et Moléculaire
Workshop – M.L. Klein Celebration (FR)

2020, 22 – 26 March – postponed to 2021
M.L. Klein Symposium at ACS Spring Meeting (USA)

2019, 28-29 November
Trends in Enzymatic Catalysis: Merging Theory and Experiments, Benicassim (SP)
Metal-Aided Enzymatic Processing of DNA and RNA

2019, 10-12 November
From Free Energy Perturbation to Biomedicine: Bridging Experiments and Computation in Chemical Biology, **Shenzhen (CH)**
Metal-Aided Enzymatic Processing of DNA and RNA

2019, 16-19 July **– Keynote speaker**
National Meeting in Medicinal Chemistry, **Milan (IT)**
Toward the computational design of nanoreceptors with intelligent recognition abilities

2019, 3-5 June
Coupled problems, Sitges, **Barcelona (SP)**
Monolayer Protected Gold Nanoparticles, on the Move: Toward Nanoreceptors with Intelligent Recognition Abilities

2019, May 8
EPFL School of Life Sciences, Lausanne (CH)
Structure-Based Drug Design, as part of the Biomolecular Structure and Mechanics course for Master students within the Institute of Bioengineering

2019, April 11
FROM - Fondazione per la Ricerca, **Ospedale di Bergamo (IT)**
Le sfide dell'innovazione tecnologica nella ricerca clinica
L'innovazione tecnologica nella discovery di nuovi farmaci

2019, March 25
University Bologna, Dept. Pharmaceutical Chemistry, Rimini (IT)
Computation for Drug Discovery

2019, February 19
Università della Calabria (IT)
Molecular modeling and simulations to investigate metalloenzymes and accelerate small-molecule drug discovery

2019, February 3-6

CECAM Workshop in Lausanne, (CH)
Multiscale Modeling from Macromolecules to Cell: Opportunities and Challenges of Biomolecular Simulations
Monolayer Protected Gold Nanoparticles, on the Move: Toward Nanoreceptors with Intelligent Recognition Abilities

2018, November 28
Structure-Based Drug Design 2018 Asia, Bali Indonesia (ID)
Molecular modeling and simulations to investigate metalloenzymes and accelerate small-molecule drug discovery

2018, Sept 28-29
Future of Enzyme Modeling – Stockholm (SE)
Metal-Aided Enzymatic Processing of DNA and RNA via Classical and Ab Initio Simulations

2018, Sept 16-20
Euroqsar2018, Thessaloniky. (GR)
Toward the computational design of nanoreceptors with intelligent recognition abilities

2018, May 9
EPFL School of Life Sciences, Lausanne (CH)
Structure-Based Drug Design, as part of the Biomolecular Structure and Mechanics course for Master students within the Institute of Bioengineering

2017, November 3-4
The CAT-ICBCS 2017 Workshop – University of Calabria (IT)
DNA and RNA processing by pharmaceutically relevant metalloenzymes: insights from multiscale simulations

2017, October 26-29 **– Keynote speaker**
ICT-HPCC17: International Conference on Theoretical and High-Performance Computational Chemistry – Hanzhou (CN).
DNA and RNA processing by pharmaceutically relevant metalloenzymes: insights from multiscale simulations

2017, September 27
Astrazeneca R&D (Göteborg, SWE)
DNA and RNA processing by pharmaceutically relevant metalloenzymes: insights from multiscale simulations

2017, August 14-18: **Opening Lecture + 2 more Lectures**
Uni. de Los Andes, Bogotà (CO)
1st Protein, Structure, Function, and Drug Discovery School
Lecture1: Paths to drug discovery and the role of computational chemistry
Lecture2: Molecular modeling and simulations for small-molecule drug discovery
Lecture3: MD simulations to investigate molecular recognition and catalysis: From DNA to nanoparticles

2017, June 22
ETH/USI – Lugano (CH) *– invited by Prof. Parrinello.*
MD simulations to investigate molecular recognition and catalysis

2017, June 11-13
Coupled Problems international conference – **Rhodes (GR)**
Session: Computational Nanomedicine I
Organization and plasticity of the nanoparticle-coating monolayer control its conformation, solubility and molecular recognition ability

2017, May 25
Vanderbilt Uni. (US)
Molecular modeling and simulations for small-molecule drug discovery

2017, May 3
EPFL School of Life Sciences, Lausanne (CH)
Structure-Based Drug Design, as part of the Biomolecular Structure and Mechanics course for Master students within the Institute of Bioengineering

2017, April 13
UCSD, Dept. Chemistry and Biochemistry, San Diego (US)
DNA and RNA processing by pharmaceutically relevant metalloenzymes: insights from multiscale simulations

2017, April, 12
Cancer Research Institute, Uni. California, **Irvine (US)**
Molecular modeling and simulations for small-molecule drug discovery

2016, Sept 13
EMBL, Grenoble (FR)
DNA and RNA processing by pharmaceutically relevant metalloenzymes: insights from multiscale simulations

2016, July 24-29
Gordon Research Conference, **Girona (ES)**
Theory and Simulation Across Scales in Molecular Science
Multiscale Molecular Simulations to Investigate Metalloenzymes of Pharmaceutical Relevance

2016, 23-25 May
Workshop CECAM, Pisa (IT)
Structural and Functional Annotation of Bioinorganic Systems: Perspectives and Challenges from Theory and Experiments
Multiscale Molecular Simulations to Investigate Metalloenzymes of Pharmaceutical Relevance

2016, April 27
EPFL School of Life Sciences, Lausanne (CH)
Structure-Based Drug Design, as part of the Biomolecular Structure and Mechanics course for Master students within the Institute of Bioengineering.

2016, May 19
Istituto di Chimica del Riconoscimento Molecolare, CNR, Milan (IT)
Multiscale Molecular Simulations to Investigate Metalloenzymes of Pharmaceutical Relevance

2015, November 24
University of Padua, Dept. Pharmaceutical Chemistry, Padua (IT)
Structure-Based Drug Design, for Master students

2015, October 8
University of Padua, Dept. Chemistry, Padua (IT)
Multiscale molecular simulations to investigate metalloenzymes of pharmaceutical relevance

2015, 28 September – 2 October
FistMat 2015 - Italian National Conference on Condensed Matter Physics (Palermo, IT)
Multiscale molecular simulations to investigate metalloenzymes of pharmaceutical relevance

2015, 26-31 September
CECAM Workshop in Julich (DE): **Computational approaches to chemical senses**
Mechanisms of lipid degrading enzymes for endogenous pain modulation

2015, 26-31 July **– Keynote speaker**
The CHITEL 2015, **Congress of Theoretical Chemists of Latin Expression, Turin (IT)**
Multiscale molecular simulations to investigate metalloenzymes of pharmaceutical relevance

2015, May 15
University of Bologna, Dept. Pharmaceutical Chemistry, Rimini (IT)
Computation for Drug Discovery

2015, April 29 – Seminar
EPFL School of Life Sciences, Lausanne (CH)

Structure-Based Drug Design, as part of the Biomolecular Structure and Mechanics course for Master students within the Institute of Bioengineering

2015, 24-26 February – **Plenary Lecture**
Computationally Driven Drug Discovery Meeting - CDDD 4th Meeting
The Angelini Research Center Auditorium, Santa Palomba, Pomezia (IT)
Multiscale molecular simulations to investigate pharmaceutically relevant enzymes

2014, October 30
Uni. de Los Andes, Dept. Chemistry, Bogotà (CO)
A multiscale approach to decipher enzymatic processing and selectivity of lipids

2014, October 29
University de Los Andes, Dept. Chemistry, Bogotà (CO)
Structure-Based Drug Design

2014, 9 September – **Key lecture**
Annual Congress of the Italian Chemical Society, Cosenza (IT)
Key lecture for the Chemistry of Biological Systems Division
Lipid Degradation in the Endocannabinoid System: Deciphering Specificity in FAAH catalysis

2014, June
University of Bologna, Bologna (IT)
Lecture for International Summer School for PhD students Functional Genomics and Drug Discovery
Computational Chemistry for Drug Discovery

2014, April
EPFL School of Life Sciences, Lausanne (CH)
Structure-Based Drug Design, as part of the Biomolecular Structure and Mechanics course for Master students within the Institute of Bioengineering

2014, February
Scuola Superiore Sant'Anna, Pisa (IT)
Structure-Based Drug Design, for PhD students

2013, December
Technical University, Munich (DE)
Structure-Based Drug Design, as part of the Protein Prediction II course for Master students within the Dept. of Informatics

2013, September
CECAM Workshop, Jülich (DE) on Coupling between protein, water, and lipid dynamics in complex biological systems: Theory and Experiments
Lipid Degradation in the Endocannabinoid System: Deciphering Specificity in FAAH catalysis

2013, July
UCL School of Pharmacy, London (GB)
From Enzymatic Function to Drug Discovery

2013, April
EPFL School of Life Sciences, Lausanne (CH)
Structure-Based Drug Design, as part of the Biomolecular Structure and Mechanics course for Master students within the Institute of Bioengineering

2013, January
German Research School for Simulation Sciences, Jülich (DE)
Identification of multitarget FAAH/COXs inhibitors: tackling inflammation with a single molecule acting on multiple proteins

2013, January
Technical University of Munich, Munich (DE)
Structure-Based Drug Design, as part of the Protein Prediction II course for Master students within the Dept. of Informatics

2013, January
Technical University of Munich, Dept. of Chemistry, Munich (DE)
Unraveling Enzymatic Function and Mechanisms of Inhibition of Pharmaceutically Relevant Targets

2012, October
University of Amsterdam, **Dept. of Chemistry, Amsterdam (NE)**
A John van Geuns lecture
Structure-based identification of multitarget FAAH/COXs inhibitors: tackling inflammation with a single molecule acting on multiple proteins

2012, May
EPFL School of Life Sciences, Lausanne (CH)
Structure-Based Drug Design, as part of the Biomolecular Structure and Mechanics course for Master students within the Institute of Bioengineering

2012, January

Technical University of Munich, Munich (DE)
Structure-Based Drug Design, as part of the Protein Prediction II course for Master students within the Dept. of Informatics

13 June 2011
Uni. Bologna, Dept. of Pharmaceutical Sciences, Bologna (IT)
Interdisciplinary rational drug design: Toward a dual-target drug for treating inflammation

2011, April
EPFL School of Life Sciences, Lausanne (CH)
Structure-Based Drug Design, as part of the Biomolecular Structure and Mechanics course for Master students within the Institute of Bioengineering

2011, January
Technical University of Munich, Munich (DE)
Structure-Based Drug Design, as part of the Protein Prediction II course for Master students within the Dept. of Informatics.

2010, June 4

University of Parma, Parma, (IT)
Workshop in: Medicinal Chemistry and Complex Systems: New Opportunities for Rational Drug Design
Effect of magnesium ion on catalytic activity of ribonuclease H

2010, June
Technical University of Munich, Munich (DE)
Structure-Based Drug Design, as part of the Protein Structure and Function Analysis course for Master students within the Dept. of Informatics

2010, April
EPFL School of Life Sciences, Lausanne (CH)
Structure-Based Drug Design, as part of the Biomolecular Structure and Mechanics course for Master students within the Institute of Bioengineering

2010, April
Uni. Bern, Bern (CH)
Structure-Based Drug Design, as part of the Methods for Biochemistry II course for Bachelor students within the Dept. of Chemistry

2009, Sept 29 – Oct 4
ICCMSE 2009 International Conference, Rhodes (GR)
Symposium Ab initio and classical molecular dynamics simulations in molecular medicine and drug desi*gn*
Enhanced Sampling Methods in Computational Drug Design

2005, March 13-17
229th ACS National Meeting, San Diego (US)
Phosphoryl Transfer Reaction in Enzymes

OTHER PRESENTATIONS AT CONFERENCES

Oral Communications

2019, August 25-29, 258th ACS National Meeting, **San Diego (US)**
Progresses in molecular dynamics simulation-directed rational design of intelligent nanoreceptors for chemosensing

2019, March-April 31-04, 257th ACS National Meeting, **Orlando (US)**
Molecular dynamics simulations to design nanoreceptors with targeted recognition abilities

2018, August 19-23, 256th ACS National Meeting, **Boston (US)**
Toward the computational design of nanoreceptors with intelligent recognition abilities

2017, April 2-6, 253rd ACS National Meeting, **San Francisco (US)**
A self-activated mechanism for efficient nucleic acids polymerization

2016, August 21-25, 252nd ACS National Meeting, **Philadelphia (US)**
Cooperative motion of a key positively charged residue and metal ions for DNA replication catalyzed by Y-family polymerases

2016, August 21-25, 252nd ACS National Meeting, **Philadelphia (US)**
HRD motif as the central hub of the signaling network for activation loop autophosphorylation in Abl kinase

2015, October 22, MINISYMPOSIUM in honor of Prof. R. Nussinov
SEMINAR in Jülich Research Center, **Jülich (DE)**
Multiscale molecular simulations to investigate metalloenzymes of pharmaceutical relevance

2015, August 16-20, 250th ACS National Meeting, **Boston (US)**
Computational and experimental insights into the spermine-vectorized F14512 poisoning of type II topoisomerase

2014, August 10-14, 248th ACS National Meeting, **San Francisco (US)**
Hydrolysis of anandamide in FAAH shows that nitrogen inversion is key to efficient enzyme-assisted amide bond cleavage

2014, August 10-14, 248th ACS National Meeting, **San Francisco (US)**
Molecular dynamics and mutagenesis studies indicate structural flexibility as a key factor for substrate specificity in FAAH catalysis

2013, April 7-11, 245th ACS National Meeting, **New Orleans (US)**
Dynamics of catalytic metals during DNA cleavage in type II topoisomerase

2013, April 7-11, 245th ACS National Meeting, **New Orleans (US)**
Structure-based identification of multitarget FAAH/COXs inhibitors: tackling inflammation with a single molecule acting on multiple proteins

2012, August 19-23, 244th ACS National Meeting, **Philadelphia (US)**
ORAL COMMUNICATION AND POSTER
Structure-based identification of multitarget FAAH/COXs inhibitors: tackling inflammation with a single molecule acting on multiple proteins

2012, April 15-17, NPCF6, **Riccione (IT)**
On binding and reactivity of potent covalent inhibitors of fatty acid amide hydrolase

2011, August 28 – September 1, 242nd ACS National Meeting, **Denver (US)**
Enzyme-induced distortion of the amide bond: A rationale for the inhibitory activity of piperidine/piperazine ureas against fatty acid amide hydrolase

2008, August 21-25, 236th ACS National Meeting, **Philadelphia (US)**

2007, August 19-24, 234th ACS National Meeting, **Boston (US)**

2006, October 12, The Chemical Biophysics Mini-Symposium on The Nature and Role of Water as a Biological Solvent, UPenn, **Philadelphia (US)**
Role of Water in Phosphatase Activity in Soluble Epoxide Hydrolase

2006, September 10-14, 232nd ACS National Meeting, **San Francisco US)**
Efficiency of Bimetal-Aided Phosphodiester Bond Cleavage in Nucleotidyl Transfer Reactions

2006, September 10-14, 232nd ACS National Meeting**, San Francisco (US)**
Water Mediated Proton Shuttles in Enzymatic Phosphoryl Transfers: Phosphatase Activity in Soluble Epoxide Hydrolase

2006, May 30, UPenn. IRG-3 seminars, **Philadelphia (US)**
Phosphoryl Transfers in Metallo-Enzymes: Insights from QM/MM Simulations

*2004, August 22-26, 228th ACS National Meeting, **Philadelphia (US)***
QM and QM/MM Studies of the Phosphoryl Transfer Reaction Catalyzed by a Cyclin-Dependent Kinase

2001, June 11-13, CECAM, **Lyon (FR)**
PsiK Workshops - Ab Initio Modelling in the Biological Sciences.
Quantum Mechanical Computational Study of Lysozyme Reaction Mechanism

Posters

2010, June 23-25, CHI's Structure-Based Drug Design Conference, **Boston (US)**

2010, March, 21-25, 239th ACS National Meeting, **San Francisco (US)**
Path collective variable and enhanced sampling methods applied to enzymatic catalysis

2010, February 26, Winter Modeling 2010, **Pisa (IT)**

2009, October 13-15, MipTec 2009, **Basel (CH)**
POSTER for The Leading European Event for Drug Discovery
5-Membered heteroaromatic rings as building blocks for RNA-binding drugs

2009, March 9-14, Gordon Research Conference, **Lucca (IT)**
New Antibacterial Discovery & Development
Two-Metal Associative Catalysis: Phosphodiester Cleavage in Ribonuclease H

2005, September 3-8, CPMD Workshop 2005, **Lugano (CH)**
Ab-initio Molecular Dynamics Simulations - from Solid State Physics to Chemistry and Biology

2003, July 14-19, ICTP, International Centre for Theoretical Physics, **Trieste (IT)**
New Frontiers in Nano-Biotechnology: Monitoring Protein Function with Single-Protein Resolution

2003, June 30 - July 4, Campus Scientifico, **Urbino (IT)**
Advanced Course of Pharmaceutical Chemistry - National Seminar E. Duranti

2002, October 7-8, **Riccione (IT)**
II S.A.Y.C.S. (Sigma Aldrich Young Chemists Symposium)

2002, August 4-9, **Lugano (CH)**
6th World Congress of Theoretically Oriented Chemists – WATOC/02

Attendee

2007, April 15-17, Schrödinger, **New York City (US)**
Spring 2007 Schrödinger User Symposium

SOCIETY MEMBERSHIPS

American Chemical Society (ACS)
Computers in Chemistry Division | Member ID: 2368275

QSAR, Cheminformatics and Modeling Society (QCMS)

Italian Chemical Society
Member of the Pharmaceutical Chemistry, Theoretical and Computational Chemistry Divisions