# MARCO D'ABRAMO

## PERSONAL INFORMATION

**Name**: Marco D'Abramo
**Birth date:** 27 October 1976
**Birth place:** Rome (Italy)
**Nationality**: Italian
**Address**: Department of Chemistry, ”Sapienza” University of Rome, P.le Aldo Moro, 5, 00185, Rome, Italy.

**E-mail**: marco.dabramo@uniroma1.it

## Curriculum Vitae

## Professional Experience

**present** → Research Fellow (r.t.d. B, tenure track), funded by “Rita Levi Montalcini” program, Department of Chemistry, Sapienza University, Rome, Italy.

Theoretical-computational studies on Homing endonuclease enzymes

**2013 to 2014** → Research fellow at CINECA, funded by “FIRB giovani” 2012. Project "Lipid based sensor for the detection of tumor biomarkers"

In-silico modeling of lipid based sensor for the detection of tumor biomarkes, in collaboration with experimental units

**2009 to 2012** → Staff Scientist in the Computational Biophysics group, Spanish National Cancer Research Center (CNIO).

I was involved in several different research projects related to cancer and other diseases:
- The effects of mutations in endonuclease protein family on the DNA cleavage (in collaboration with the Macromolecular Crystallography group @CNIO).
- Development of new algorithms to sample rare events in order to address pharmacologically relevant processes as protein-ligand binding (in collaboration with the CNIO Experimental Therapeutics section).
- Setup of a computational framework to predict and clarify the role of key residues in kinases coupling bioinformatics data with very long molecular dynamics simulations (in collaboration with Structural Computational Biology group @ CNIO).
- Kinetics of charge transfer in single and double stranded DNA for its use in biophysics and nanotechnology

**2007 to 2009** → Post-doc position in the Molecular Modeling & Bioinformatics group of Prof. Modesto Orozco, (Parc Cientific De Barcelona) Institute of Research in Biomedicine, Barcelona, Spain.

**2007 to 2007** → Post-doc position in the Barcelona Supercomputing Center.

My research topics were:
- The characterization of proteome dynamics in different environments by means of molecular dynamics simulations.
- The improvement of protein structure predictions by coupling low-resolution data with molecular dynamics and docking algorithms
- Theoretical characterization of peptide nanotubes to explore their use as molecular carriers
- Modeling of DNA electronic properties for biophysics and nanotechnology applications

**Nov 2005 – Mar 2006** Visiting Student in the Molecular Modeling & Bioinformatics group of Prof. Modesto Orozco, founded by the European Project "High Performance Computing". Title of the project "Characterization of the CO kinetics in myoglobin".

## Scientific Education

**2003-2006** PhD fellowship in Chemistry Sciences at the Universita' degli Studi di Roma "La Sapienza", Roma, Italia. Research project: "Statistical mechanics of complex molecular systems". Supervisors A. Amadei and A. Di Nola

**2003** Degree (Laurea) in Chemistry at the Universita' degli Studi di Roma "La Sapienza". Supervisor A. Amadei and A. Di Nola. Thesis: "Thermodynamic properties of infinite diluted solutions".

## Research interests summary

My main research interest concerns the study of the electronic, thermodynamic and structural properties of complex systems combining computational methods and advanced molecular theories.
I have active international collaborations with top-groups in the field of X-ray crystallography, NMR, Small-X-ray Scattering and Molecular Biology where the "in-silico" modeling of the experiment is used to elucidate key-steps of the reaction mechanisms and to propose nontrivial explanations of the experimental findings. At present, my main research lines concern the theoretical modeling of the endonuclease behavior, the study of the intracellular part of the T-Cell receptor by computational methods as well as the structural and dynamical characterization of protein evolutionary pathway.

## Teaching Activity

- **2016/2017** Teaching Course: Chemistry, Geological Sciences degree course, Sapienza University of Rome (Italy).
- **2015/2016** Teaching Course: Chemistry, Geological Sciences degree course, Sapienza University of Rome (Italy).
- **2014/2015** Teaching Course: Chemistry, Geological Sciences degree course, Sapienza University of Rome (Italy).
- **2006** *Teaching Assistant: MASTER in "Bioinformatica: applicazioni biomediche e farmaceutiche"*, Biochemistry Department "A. Rossi Fanelli", University of Rome "La Sapienza" (Italy)

- **2005** *Teaching Assistant: MASTER in "Bioinformatica: applicazioni biomediche e farmaceutiche"*, Biochemistry Department "A. Rossi Fanelli", University of Rome "La Sapienza" (Italy)

- **2003-2005** *Teaching Assistant: Courses: 'Computational Chemistry', 'Elements of Chemical Informatics', 'Mathematics'*. Chemistry Department, University of Rome "La Sapienza" (Italy).

- **2004** *Teaching Assistant (Excercises): MASTER in "Bioinformatica: applicazioni biomediche e farmaceutiche"*, Biochemistry Department "A. Rossi Fanelli", University of Rome "La Sapienza" (Italy)

**Thesis Supervisor**

- **2015** Bachelor Degree (Chemistry). Simone Cecconi. Thesis Title: "Caratterizzazione del comportamento conformazionale della Endonucleasi I-DmoI attaverso simulazioni di Dinamica Molecolare".

- **2015-2016** Master Degree (Pharmacy). Josephine Alba. Thesis Title: "Studio del comportamento conformazionale della endonucleasi I-DmoI in presenza del DNA attraverso simulazioni di Dinamica Molecolare".

- **2016-** Master Degree (Pharmacy). Alexandra Trandafir. Thesis Title: "Studio dei Cambiamenti conformazionali nelle chinasi di tipo Src attraverso l'uso di algoritmi avanzati di Dinamica Molecolare".

## Publications

Total Documents: 52

Citations: 624

h-index: 15

Co-authors: 109

(source: Scopus 20/09/2016)

***Book chapter***

David Piedra, Marco D'Abramo and Xavier de la Cruz **(2011)**. Contributions of Structure Comparison Methods to the Protein Structure Prediction Field, Computational Biology and Applied Bioinformatics, ISBN: 978-953-307-629-4, **InTech**, DOI: 10.5772/21052.

***Articles***

*51. Grottesi, A., Cecconi, S., Molina, R., D'Abramo, M.*

Effect of DNA on the Conformational Dynamics of the Endonucleases I-DmoI as provided by molecular dynamics simulations

***Biopolymers**, DOI: 10.1002/bip.22933* ***(2016)***

*50. D'Abramo, M., Bešker, N., Desideri, A., Levine, A.J., Melino, G., Chillemi, G.*

The p53 tetramer shows an induced-fit interaction of the C-terminal domain with the DNA-binding

domain

**Oncogene**, 35 (25), pp. 3272-3281 **(2016)**.

49. *Chillemi, G., Pace, E., D'Abramo, M., Benfatto, M.*

    *Equilibrium between 5- and 6-fold coordination in the first hydration shell of Cu(II)*

    **Journal of Physical Chemistry A**, 120 (22), pp. 3958-3965 **(2016).**

48. *Molina, R., Besker, N., Marcaida, M.J., Montoya, G., Prieto, J., D'Abramo, M.*

    Key Players in I-DmoI Endonuclease Catalysis Revealed from Structure and Dynamics

    ***ACS Chemical Biology**, 11 (5), pp. 1401-1407 **(2016)**.*

47. *Petaccia, M., Gentili, P., Bešker, N., D'Abramo, M., Giansanti, L., Leonelli, F., La Bella, A., Gradella Villalva, D., Mancini, G.*

    Kinetics and mechanistic study of competitive inhibition of thymidine phosphorylase by 5-fluoruracil derivatives

    **Colloids and Surfaces B: Biointerfaces**, 140, pp. 121-127 ***(2016)***.

46. *Del Galdo, S., Marracino, P., D'Abramo, M., Amadei, A.*

    *In silico characterization of protein partial molecular volumes and hydration shells*

    **Physical Chemistry Chemical Physics**, 17 (46), pp. 31270-31277 **(2015)**.

45. *Mauceri, A., Fracassi, A., D'Abramo, M., Borocci, S., Giansanti, L., Piozzi, A., Galantini, L., Martino, A., D'Aiuto, V., Mancini, G.*

    Role of the hydrophilic spacer of glucosylated amphiphiles included in liposome formulations in the recognition of Concanavalin A

    **Colloids and Surfaces B: Biointerfaces**, 136, pp. 232-239 ***(2015)***.

44. *D'Abramo, M., Aschi, M., Amadei, A.*

    Theoretical calculation of the pyrene emission properties in different solvents

    **Chemical Physics Letters**, 639, pp. 17-22 **(2015)**.

43. *Molina, R., M.J. Marcaida, P. Redondo, M. Marenchino, P. Duchateau, M. D'Abramo, G. Montoya, J. Prieto*

    Engineering a Nickase on the Homing Endonuclease I-DmoI Scaffold

    ***J. Biol. Chem.,** 290 (30) **(2015),***

42. *M. Barbany; T. Meyer; A. Hospital; I. Faustino; M. D'Abramo; J. Morata; M. Orozco; X. de la Cruz*

    Molecular Dynamics Study of Naturally Existing Cavity Couplings in Proteins

    **Plos One**, e0119978 *(10)* ***(2015)***

41. *N. Bešker, A. Amadei, M. D'Abramo**

    Molecular mechanisms of activation in CDK2

    **J. of Biomol. Struct. Dyn.,** dx.doi.org/10.1080/07391102.2013.844080 ***(2014)***

40. *G. Piacente, A. Amadei, M. D'Abramo, I. Daidone, M. Aschi*

    Theoretical-computational modeling of photo-induced charge separation spectra and charge recombination kinetics in solution.

    ***Phys. Chem. Chem. Phys. ISSN:1463-9076 vol. 16 (2014)***

39. *M. D'Abramo*, N. Bešker, G. Chillemi, A. Grottesi*

    Modeling conformational transitions in kinases by molecular dynamics simulations: achievements, difficulties, and open challenges

    **Frontiers in Genetics,** *5:128* ***(2014)***

38. *M. D'Abramo, M. Aschi, A. Amadei*

Theoretical modeling of UV-Vis absorption and emission spectra in liquid state systems including vibrational and conformational effects: Explicit treatment of the vibronic transitions
***J. Phys. Chem.*** 28;140(16):164104 ***(2014)***

37. *Chillemi G, Davidovich P, D'Abramo M, Mametnabiev T, Garabadzhiu AV, Desideri A, Melino G.*
Molecular dynamics of the full-length p53 monomer.
**Cell Cycle,** 12(18):3098-108 ***(2013)***

36. *D'Abramo, M., Castellazzi, C.L., Orozco, M., Amadei, A.*
On the nature of DNA hyperchromic effect
***J. Phys. Chem. B*** *117 (29) , pp. 8697-8704* ***(2013)***

35. *Molina, R., Redondo, P., Stella, S., Marenchino, M., D'Abramo, M., Gervasio, F.L.c, Charles Epinat, J., Valton, J., Grizot, S., Duchateau, P., Prieto, J. , Montoya, G.*
Non-specific protein-DNA interactions control I-CreI target binding and cleavage
***Nucleic Acids Research*** *40 (14) , pp. 6936-6945* ***(2012)***

34. D'Abramo, M., Rabal, O., Oyarzabal, J., Gervasio, F.L.
Conformational selection versus induced fit in kinases: The case of PI3K-γ
**Angewandte Chemie - International Edition** 51 (3) , pp. 642-646 ***(2012 )***

33. *M. D'Abramo*, M. Orozco, A. Amadei*
Effects of local electric fields on the redox free energy of single stranded DNA
**Chem. Comm.** DOI: 10.1039/C0CC04352D ***(2011)***

32. *L. Sutto, M. D'Abramo, F.L. Gervasio*
Comparing the efficiency of biased and unbiased molecular dynamics in reconstructing the free energy landscape of Met-enkephalin.
**J. Chem. Theo. Comp.,** *6 (12), 3640-3646* ***(2010)***

31. *M D'Abramo, T. Meyer, A. Hospital, M. Rueda, C. Ferrer-Costa, A. Pérez, O. Carrillo, J. Camps, C. Fenollosa, D. Repchevsky, J.L. Gelpí, M. Orozco*
MoDEL (Molecular Dynamics Extended Library): A database of atomistic molecular dynamics trajectories
**Structure,** 18(11), 1399-1409 ***(2010)***

30. *C. Pons, M. D'Abramo, D.I. Svergun, M. Orozco, P. Bernadó, J. Fernández-Recio*
Structural characterization of protein-protein complexes by integrating computational docking with small-angle scattering data.
**J. Mol. Biol.,** *403, 217-230* ***(2010)***

29. *I. G. Muñoz, J. Prieto, S. Subramanian, J. Coloma, P. Redondo, M. Villate, N. Merino, M. Marenchino, M. D'Abramo, F.L. Gervasio, S. Grizot, F. Daboussi, J. Smith, I. Chion-Sotinel, F. Pâques, P. Duchateau, A. Alibés, F. Stricher, L. Serrano, F.J. Blanco, G. Montoya*
Molecular basis of engineered meganuclease targeting of the endogenous human RAG1 locus
**Nucleic Acids Res.** *39 (2): 729-743* ***(2010)***

28. *M. D'Abramo, T. Meyer, P. Bernadó, C. Pons, J.F. Recio, M. Orozco*
On the Use of low-resolution Data to Improve Structure Prediction of Proteins and Protein Complexes
**J. Chem. Theo. Comp.,** *5, 3129-3137* ***(2009)***

27. *Marco D'Abramo*, Massimiliano Aschi, Andrea Amadei*
Charge transfer equilibria of aqueous single stranded DNA.
**PhysChemChemPhys** *11 (45) 10614-8****(2009)***

26. *R. García-Fandiño, J. R. Granja, M. D'Abramo*, M. Orozco*
Theoretical characterization of the dynamical behavior and transport properties of alpha,gamma-peptide nanotubes in solution.

**J. Am. Chem. Soc.** 131 (43) p. 15678-86 **(2009)**

25. *M. D'Abramo, A. Di Nola and Andrea Amadei*

    The kinetics of carbon monoxide migration and binding in solvated myoglobin as revealed by molecular dynamics simulations and quantum mechanical calculations

    **J. Phys. Chem. B** 113, 16346-16353 **(2009)**

24. *A. Amadei, M. D'Alessandro, M. D'Abramo and M. Aschi*

    Theoretical characterization of electronic states in interacting chemical systems

    **J. Chem. Phys.** 130(8), 08410 **(2009).**

23. *J. Camps, O. Carrillo, A. Emperador, L. Orellana, A. Hospital, M. Rueda, D. Cicin, M. D'Abramo, J. L. Gelpí and M. Orozco*

    FlexServ: An integrated tool for the analysis of protein flexibility

    **Bionformatics** 25 (13) p. 1709-10 **(2009)**

22. *M. D'Abramo, R. Caminiti, A. Di Nola and A. Amadei*

    What can we learn by comparing experimental and theoretical-computational X-ray scattering data?

    **J. Mol. Liq.** 144(*1-2*), *9-12* **(2009)**

21. *F. Apollonio, M. Liberti, A. Amadei, M. Aschi, M. Pellegrino, M. D'Alessandro, M. D'Abramo, A. Di Nola and G. d'Inzeo*

    Mixed Quantum-Classical Methods for Molecular Simulations of Biochemical Reactions With Microwave Fields: The Case Study of Myoglobin

    **Microwave Theory and Techniques, IEEE Transactions on** 56(11), 2511-2519 **(2008).**

20. *M. D'Abramo, A. Di Nola, M. Aschi and A. Amadei*

    Theoretical characterization of temperature and density dependence of liquid water electronic excitation energy: Comparison with recent experimental data.

    **J. Chem. Phys.** 122, 154109 **(2008).**

19. *M. Aschi, M. D'Alessandro, M. Pellegrino, A. Di Nola, M. D'Abramo and A. Amadei*

    Intramolecular charge transfer in π-conjugated oligomers: a theoretical study on the effect of temperature and oxidation state.

    **Theor. Chem. Acc.** 119(5-6), 469-476 **(2008).**

18. *A. Amadei, M. D'Abramo, A. Di Nola, A. Arcadi, G. Cerichelli and M. Aschi*

    Theoretical study of intramolecular charge transfer pi-conjugated oligomers.

    **Chem. Phys. Lett.** 434(4-6), 194-199 **(2007)**.

17. *A. Amadei, M. D'Abramo, I. Daidone, M. D'Alessandro, A. Di Nola and M. Aschi*

    Statistical mechanical modeling of chemical reactions in complex systems: the kinetics of the haem carbon monoxide binding-unbinding reaction in myoglobin.

    **Theor. Chem. Acc.** 117(5-6), 637-647 **(2007)**.

16. *M. D'Abramo, M. Aschi, F. Marinelli, A. Di Nola and A. Amadei*

    Theoretical prediction of thermodynamic equilibrium constants of chemical reactions in water.

    **J. Mol. Struc.-Theochem.** 811(1-3), 197-201 **(2007)**.

15. *C. Zazza, A. Amadei, N. Sanna, A. Grandi, G. Chillemi, A. Di Nola, M. D'Abramo and M. Aschi*

    Theoretical modeling of the valence UV spectra of 1,2,3-triazine and uracil in solution.

    **Phys. Chem. Chem. Phys.** 8, 1385-1393 **(2006)**.

14. *M. D'Abramo, M. Aschi, A. Di Nola and A. Amadei*

    On the importance of configurational sampling in theoretical calculation of electronic properties of complex molecular systems: acetone in water.

    **Chem. Phys. Lett.** 424(4-6), 289-294 **(2006)**.

13. *M. D'Abramo, M. C. Rinaldi, A. Bozzi, G. Mignogna, A. Di Nola, A. Amadei and M. Aschi*

Conformational behavior of Temporin A and Temporin L in aqueous solution: a computational/experimental study

**Biopolymers**, 81(3), 215-224, **(2006)**.

12. *Apollonio, F., D'Abramo, M., Liberti, M., Amadei, A., Di Nola, A., D'Inzeo, G.*

Myoglobin as a case study for molecular simulations in the presence of a microwave electromagnetic field

**IEEE MTT-S International Microwave Symposium Digest** , 4015287 , pp. 1746-1749 **(2006)**

11. *M.Aschi , M. D'Abramo, F. Ramondo, I. Daidone, M. D'Alessandro, A. Di Nola and A. Amadei*

Theoretical modeling of chemical reactions in complex environments: the intramolecular proton transfer in aqueous malonaldehyde.

**J.Phys.Org.Chem.** 19, 518-530 **(2006)**.

10. *M. D'Alessandro, M. D'Abramo, M. Paci and A. Amadei*

Theoretical Study of the Thermodynamics of a Solvated Peptide: Contryphan Vn.

**Physica Scripta** T118, 196, **(2005)**.

9. *I. Daidone, M. D'Abramo, A. Di Nola and A. Amadei*

Theoretical characterization of alpha-helix and beta-hairpin folding kinetics.

**J. Am. Chem. Soc.** 127(42), 14825-14832, **(2005)**.

8. *M. D'Alessandro, F. Marinelli, M. D'Abramo, M. Aschi, A. Di Nola and A. Amadei*

Ground and excited electronic state thermodynamics of aqueous carbon monoxide: a theoretical study.

**J. Chem. Phys.** 122, 124507 **(2005)**.

7. *A. Amadei, F. Marinelli, M. D'Abramo, M. D'Alessandro, M. Anselmi, A. Di Nola and M. Aschi*

Theoretical modeling of vibro-electronic quantum states in complex molecular systems: solvated carbon monoxide, a test case.

**J. Chem. Phys.** 122, 124506 **(2005)**.

6. *M. Aschi, M. D'Abramo, C. Di Teodoro, A. Di Nola and A. Amadei*

Theoretical characterization of liquid water electronic excitation.

**ChemPhysChem.** 6(1), 53-58 **(2005)**.

5. *M. D'Abramo, M. Aschi, A. Di Nola, A. Amadei*

Calculation of the Optical Rotatory Dispersion of solvated alanine by means of the Perturbed Matrix Method.

**Chem. Phys. Lett.** 402, 559-563 **(2005).**

4. *M. D'Abramo, M. D'Alessandro, A. Di Nola, D. Roccatano and A. Amadei*

Characterization of liquid behavior by means of local density fluctuations.

**J. Mol. Liq.** 117, 17-21 **(2005)**.

3. *M. D'Abramo, M. D'Alessandro and A. Amadei*

On the use of the quasi Gaussian entropy theory in the study of simulated dilute solutions.

**J. Chem. Phys.** 120, 5526-5531 **(2004)**.

2. *A. Amadei, M. D'Abramo, C. Zazza and M. Aschi*

Electronic properties of Formaldehyde in water: a theoretical study.

**Chem. Phys. Lett.**, 381, 187- 193 **(2003)** .

1. *M. D'Alessandro, M. D'Abramo, G. Brancato, A. Di Nola and A. Amadei*

Statistical mechanics and thermodynamics of simulated ionic solutions.

**J. Phys.Chem. B** 106 (45), 11843-11848 **(2002)**.

## Conferences and Workshops

- **2016** Protein Structural Dynamics: Biological Systems and Experimental strategies, Rome, Italy.
- **2015** Chiritaly, Rome, Italy.
- **2015** CINECA, Scuola di Dinamica Molecolare, Roma, Italia.
- **2015** (Organizing Commitee) III Congresso della Società Chimica Italiana, divisione di Chimica Teorica e Computazionale.
- **2014** Solutions for Solvation, Pisa, Italia (2014)
- **2014** Poster. Eleventh Annual Meeting of the Bioinformatics Italian Society, Rome, Italy.
- **2014** Poster. Proteine 2014, Padua, Italy.
- **2013** Oral Communication. Computational approaches applied to chemical and biochemical processes. Vignale Monferrato, Italy.
- **2010** Oral Communication. Exascale Challenges in Computational Biology. Barcelona
- **2009** Oral Communication. Collaborative Computational Project for Biomolecular Simulation (CCPB). York, UK**.**
- **2008** Grand Challenges in Computational Biology. Barcelona, Spain.
- **2008** Oral Communication. 7th workshop on molecular theory and simulations. Gaeta, Italy.
- **2008** Oral Comunication. XI Encuentro Peptidico Iberico. Santiago de Compostela, Spain.
- **2008** Poster JNB'08 VIII Jornadas de Bioinformática. Valencia, Spain
- **2007** BSC-IRB Barcelona Conference on Computational Biology: Biomolecular Simulations, Bioinformatics and Supercomputing. Barcelona, Spain
- **2007** Oral Communication 6th workshop on molecular theory and simulations. Gaeta, Italy.
- **2006** Oral Communication 5th workshop on molecular theory and simulations. Gaeta, Italy.
- **2006** Oral Communication Trans Mobility Access Meeting. Barcelona, Spain.
- **2005** Oral Communication 4th workshop on molecular theory and simulations. Gaeta, Italy.
- **2004** Poster Math/Chem/Comp: "The Nineteenth International Course & Conference on the Interfaces among Mathematics, Chemistry & Computer Sciences". Dubrovnik, Croatia.
- **2004** Oral Communication 3rd workshop on molecular theory and simulations. Gaeta, Italy.
- **2003** Oral Communication 2nd workshop on molecular theory and simulations. Gaeta, Italy.
- **2003** Poster Euresco Conferences: "Routes from Local Order to Large-Scale Cooperativity". Lucca, Italy.

- **2002** Poster NATO-ASI Summer school on physical-chemistry of liquids: "Novel Approaches to the Structure and Dynamics of Liquids: Experiments, Theories, Simulations". Rodi, Greece

## Fundings

- **2017** “Torno Subito”, Regione Lazio (**Host Laboratory** for pre-doctoral fellow, 6 months).
  Project Title: Molecular mechanisms of T-Cell activation

- **2016** ZIP Solutions, private company **(PI)**.
  Project Title: In-silico characterization of inteins: structure, dynamics and interaction behavior.

- **2015** Visiting Professor, Sapienza University of Rome **(Host Laboratory)**.
  Description: Structural-dynamical study of the Src kinase activity

- **2015** Research Project, Sapienza University of Rome **(PI)**.
  Project Title: Combined approach of computational methods and experimental techniques for the characterization of the molecular basisi of the inhibition of the MKK7-GAD complex by means of tripeptides.

- **2014** Research Project, Sapienza University of Rome (Participant).
  Project Title: Theoretical Modelling of Ionic Liquids.

- **2014** Rita Levi Montalcini fellowship, Italian Ministry of Research and Education, (3 years, **PI**).
Project Title: Theoretical modelling of Endonucleases.

- **2013** Firb Giovani, Italian Ministry of Research and Education(3 years, **PI of the Computational Unit**).
Project Title: Lipid based sensor for the detection of tumor biomarkers.

- **2012** HPC2 Europa Project, EU (3 months, **PI**).

- **2009** “Miguel Servet” fellowship, Spanish Ministry of Research and Innovation (5 years, **PI**).
Project Title: Computational study of Endonucleases.

- **2007** Foreigners post-doc fellowship, Spanish Ministry of Research and Innovation.
Project Title: Computational modelling of DNA electronic properties, funded by, (15 months).

- **2006** HPC Europa Project, EU (3 months, **PI**).

## Other Academic Activities

- Maintenance (software and hardware) and management of the local High-Performance Computing cluster “Narten”.

- Recipient of computational time grants issued by CINECA by competitive calls. ISCRA B 2015, ISCRA B 2016, ISCRA B 2015 (totalling about 2 Millions core hours).

- Recipient of GPU Grant Program (1 Titan-X GPU).

- **Abilitazione Scientifica Nazionale** (National Academic Qualification as Associate Professor) 03/A2 – II fascia. 29/01/2014-29/01/2020.

Date

Signature