DOTT. ROBERTA GALEAZZI

CURRICULUM VITAE- English short version

Education and Training

Dr. Roberta Galeazzi got the Chemistry degree in 1992 at the University of Bologna *cum laude* and worked as researcher since January 1993 at the Polytechnic Marche University (Università Politecnica delle Marche), where actually she is assistant professor of the Department of Life and Environmental Science (DISVA). Dr. Galeazzi actually is the leader of the BioMolecular Modeling group (bioMM) and scientific director of the molecular Modeling Laboratory (MMLab). The bioMM group research focus on molecular modelling and its applications in chemistry and biology. Recent research achievements concern the application of atomistic Molecular dynamics to the study of the conformational and structural characterization of complex supra-macromolecular systems such as membrane receptors (ex. 5-HT2c) and mixed composition membrane lipid bilayers as vectors for Gene-Delivery and Drug Design.

Since a.a.2001-2002 , she teaches many courses for the degree in Biology and for the master course of Molecular and Applied Biology (*Biomolecular Modeling* and *Receptorial Chemistry; actually Modeling of Biological Systems).*

Furthermore since 2005 she is a member of the PhD course in *Biomolecular Applied Science*, now PhD School of DISVA, where she also teach a course in *Advanced Biomolecular Modeling*.

She is co-author of 80 papers published on international peer-review journals and she attended to many congresses with oral and poster presentations. She has been also reporter and co-reporter of many molecular modelling experimental thesis for the Faculty of Science and tutor of PhD thesis for the PhD School of Science Faculty in Biomolecular science.

She has got granted as P.I. several Peer-review projects both at national and European level. Among them, she had accessed till 2008 to ISCRA CINECA resources granting:

-High Performance Computing (HPC) projects at CINECA (FERMI Blue-Gene, SP6 e PLX workstations) ISCRA call C (2008-2017)

- European **HPC approved projects** (PRACE DECI grants 2012-2013 http:// www.prace-ri.eu).

She is actually a member of the direction board for the Italian Chemistry Society (section Marche).

She is guest editor of a special issue in Molecules (MDPI journal) in Biomolecular simulations.

She is curenlty a reviewer for many relevant journals in such as Current Computer Aided Drug Design (CCADD) , Journal of Computational Chemistry, Journal of Molecular Modeling, ACS Journal of Chemical Theory and Computation (JCTC), Molecules, Expert opinion in Drug Discovery, Anticancer Agent in Medicinal Chemistry.

Research Activity

Dr Galeazzi's main research activity concerns molecular docking and molecular dynamics profiling of novel active compounds or natural ligands to their receptors with the aim of rationalize the molecular basis of biological processes fundamental for the transductions of specific biochemical and physiological effects. Most of research activity concerns the application of Molecular Docking

and Molecular Dynamics to the activity prediction of natural ligands/novel active compounds to their target receptors. Moreover, the research efforts are directed towards the elucidation of the molecular basis of biological processes involved in the transductions of specific biochemical and physiological effects. In MMLab, researcher uses a broad range of up-to-date modeling packages such as AMBER, GROMACS, Autodock, CHIMERA, VMD/NAMD.
The study of this molecular aspect extends also to the computational investigations of enzymatic mechanisms using DFT methods combined with MD simulations onto the reaction PES.
Some research achievements concerns to application of full atom Molecular dynamics to the study of the conformational and structural characterization of complex supra-macromolecular systems such as membrane receptors (ex. 5-HT2c serotonin receptor) and membrane lipid bilayers in mixed composition able or to complex DNA (Gene-Delivery) or to deliver drugs to the cellular target (Drug-Delivery systems).

Research Activity: The research activity is oriented towards biomolecular modelling and computational chemistry; In particular, one of these field is molecular modelling of electronic and thermodynamic properties (by using both molecular mechanic and quantum mechanical methods (*ab initio* and DFT)) joint to conformational analysis (by means of Molecular Dynamics using both solvent explicit and implicit models) of biomolecules or bioactive compounds.

At present, one of the major field of interest is molecular docking and virtual screening of novel active compounds or natural ligands to their receptors combining both automated docking and molecular dynamics simulations, with the aim of rationalizing the molecular basis of biological processes fundamental for the transductions of specific biochemical and physiological effects. The study of this molecular aspect has also been extended to the computational investigations of enzymatic mechanisms using DFT methods combined with MD simulations onto the reaction PES. To this purpose she currently uses a broad range of computational chemistry packages such as AMBER, Gaussian09, GROMACS, Autodock.

As an application, in the last few years a particular attention have been directed to application of full atom Molecular dynamics to the study of the conformational and structural characterization of complex supra-macromolecular systems such as membrane receptors (ex. 5-HT2c serotonin receptor) and membrane lipid bilayers in mixed composition able or to complex DNA (gene-delivery) or to deliver drugs to the cellular target (Drug-Delivery systems).

She has got access to High Performance Computing (HPC) at CINECA (FERMI Blue-Gene, SP6, PLX and EURORA workstations) after approved projects grants (**peer-review**) HPC ISCRA (2008-2014) (http://www.hpc.cineca.it/services/iscra), Europeans **HPC** (PRACE DECI grants 2012 http://www.prace-ri.eu).