Supervisor Project Idea

Supervisor

Prof. Roberta Galeazzi
Associate Professor in Organic Chemistry
National Scientific Qualification for Full professor in Organic Chemistry
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- 130 scientific papers published in international peer review Journals
- More than 100 participations to National/international meetings
- H index 29 (Scopus), 32(Google Scholar)
- Citations 2282 (Scopus), 2811 (Google scholar)

Head of the Molecular Modeling Laboratory (MMLab) at Department of Life and Environmental Sciences (DISVA)
Main research focuses: 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 and mixed composition lipidic nanovectors for Gene and Drug Delivery.
Main Peer-review projects granted as P.I.

- UNIVPM unit FISR -MIUR, 2021; MISMA for Covid-19. FISR2020IP_04831
- EUROPEAN FACILITY PROJECTS PRACE DECI-9 HPC, acronym DOPE; Molecular Dynamics simulations of mixed DOPC/DOPE based membrane bilayer
- High Performance Computing (HPC) projects at CINECA (M100, Galileo, FERMI Blue-Gene, SP6 e PLX workstations) ISCRA call C (from 2008 to 2023).

Partecipant PNNR project VITALITY (2023-2026) Design of Bionanovectors for Drug Delivery and Phyotchemicals.
Member of the direction board for the Italian Chemistry Society (section Marche) from 2014 to 2020.
Editor for Molecular Informatics section of international Journal of Molecular Science.

5 latest relevant papers:

1. R. Galeazzi* and F. Costa, G.Giorgini, C. Minnelli, G. Mobbili, C. Guardiani, A.Giacomello, Membrane Composition Allows the Optimization of Berberine Encapsulation in Liposomes. Mol. Pharmaceutics, 2024, 21, 11, 5818
2. R. Galeazzi* and G. Giorgini, A. Di Gregorio, G. Mangiaterra, N. Cedraro, C. Minnelli, G.Sabbatini, G. Mobbili, S.Simoni, C. Vignaroli, Inhibition of polymorphic MexXY-OprM efflux system in Pseudomonas aeruginosa clinical isolates by Berberine derivatives, ChemMedChem,2024, 19, e202300568
3. Galeazzi, R*., and Laudadio, E., Minnelli, C., Mobbili, G., Sabbatini G., Stipa P., Rusciano, D., Salt effects on mixed composition membranes containing an antioxidant lipophilic edaravone derivative: a computational-experimental study, Org Biomol Chem, 2022, 20, 5784
4. R. Galeazzi*, and L. Massaccesi, E. Laudadio, C. Minnelli, G.Mobbili, Cholesterol-mediated oligomerization pathways of serotonin G-coupled receptor 5-HT2C, IJ Biol Macromolecules, 2020, 160, 1090
5. Galeazzi R.*, and Minnelli C., Laudadio E., Mobbili G., Conformational Insight on WT- and Mutated-EGFR Receptor Activation and Inhibition by Epigallocatechin-3-Gallate: Over a Rational Basis for the Design of Selective Non-Small-Cell Lung Anticancer Agents, Int. J. Mol. Sci, 2020, 21, 1721

Research Group Description

Prof. Galeazzi is the leader of the Molecular Modeling and Drug Design group (MMDD) and scientific director of the molecular Modeling Laboratory (MMLab). The MMDD group is composed by postdoctoral fellows and master thesis students; main research focus is on molecular modelling and its applications in chemistry and biology.

Main research activity: 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

The study of this molecular aspect has also been extended also to the computational investigations of enzymatic mechanisms using DFT methods.

Some research achievements concern to application of Molecular dynamics to the study of the conformational and structural characterization of complex supra-macromolecular systems such as membrane receptors (GPCRs i.e 5HT-2c, 5-HT1A. hMT1-hMT2) 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).

Laboratory facilities: N.2 Workstations GPU based with NVIDIA GEFORCE RTX 3070 (winblu i7 Expert Z490 10TH) and RTX 4070 SUPER (AMD RYZEN 9 7900 (3.7 GHz)- SSD nVme 1TBRAM- DDR5 64GB – liquid cooler - GEFORCE RTX 4070 SUPER 12GB; other three ubuntu workstations NVIDIA GPU based i5/i7 intel. Software Licenses for docking and Dynamics Packages (Autodock, GROMACS, AMBER, Autodock Vina GPU, VMD/NAMD, G16).

HPC access to HPC (High Performance Computing) server at DISVA, based on AMB EPYC 7301 CPU 16-Core processor

External links:

- www.mmddlab.org
- MMDDLab Web page Facebook

Research thematic area

MSCA Panel Chemistry (CHE) - Economic sciences (ECO) - Information Sciences and Engineering (ENG) - Environmental and Geosciences (ENV) - Life Sciences (LS) - Mathematics (MAT) - Physics (PHY) - Social Sciences and Humanities (SOC)	**MSCA Keywords** MSCA Panels & Keywords.pdf Link documento	**Free keywords**	**Free text**
Chemistry (CHE)	C2: Molecular Chemistry	Molecular dynamics	
	C2: Organic Chemistry	Computer Aided Drug Design	
	C3: Physical Chemistry of biological systems; Quantum Chemistry	Molecular bilayers simulations	
Life Science (LS)	L2: Computational Biology	Comparative Molecular Modeling	

	L2: Computational Biology	GPCR membrane receptors	

Contact details

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OPTIONAL:
Title and goals

Title:Mechanistic Insight on Nurr1 agonists as dopaminergic pathway activators: toward a personalized strategy in the Parkinson Disease and other neurological disorders (MINA)
Supervisor: Prof. Roberta Galeazzi

Parkinson's disease (PD) is the second most prevalent neurodegenerative disorder after Alzheimer's disease, characterized by the selective degeneration of midbrain dopamine neurons (mDANs) in the substantia nigra. The onset of PD is influenced by both environmental and genetic factors. Damage to the central dopaminergic system results in motor and learning impairments, directly linked to the degeneration of dopaminergic neurons. Nurr1, a transcription factor, is crucial for dopamine production and mDANs maintenance; this make it an important target for a successful therapeutic approach. The use of up-to-date computational methods has a high innovation potential to approach this objective in a faster and more direct approach.

Main objectives:
1. Nurr1 binding sites analysis and elucidation of its activation mechanism
2. Identification of ready-to-use Nurr1 agonists from the FDA approved drugs or the Natural pool
3. Full structure elucidation of the canonical and all the polymorphisms associated to neurological diseases such es Parkinson and Schizophrenia.
4. Assessments of Nurr1 agonists towards known polymorphic receptor