

CURRICULUM VITAE

DR ROSA MARIA VITALE (ICB-CNR)

WORK EXPERIENCE

Dates (from – to)

2007- present Permanent Researcher at Biomolecular Chemistry Institute (ICB), National Research Council (C.N.R.), Italy

2005-2007 Researcher TD art. 23 at Biostructure and Bioimaging Institute (IBB), National Research Council (C.N.R.), Italy

2004-2005 Researcher TD art. 15 at Biostructure and Bioimaging Institute (IBB), National Research Council (C.N.R.), Italy

2003-2004 Research activity at Biostructure and Bioimaging Institute (IBB), National Research Council (C.N.R.), Italy

2002-2003 Research activity at Telethon lab of Prof. Francesca Fanelli, University of Modena and Reggio Emilia

1999 Research Activity at Computational Chemistry lab of Prof. Pier Giuseppe De Benedetti, University of Modena and Reggio Emilia.

1998-1999 Research activity at Computational Chemistry lab of Prof. Carlo Pedone, University "Federico II" of Naples

EDUCATION AND TRAINING

Dates (from – to)

1997-2000/2003-2004

Name and type of organisation providing education and training

Faculty of Mathematics, Physics and Natural Science of University Sciences, University "Federico II" of Naples

Principal subjects occupational skills covered

Post-graduated Specialization's degree in "Biotechnological Applications"

Title of qualification awarded

Specialization's Degree (70/70 cum laude)

Level in National classification

I classified and fellowship winner

Dates (from – to)

2000-2003

Name and type of organisation providing education and training

Faculty of Environmental Sciences, II University of Naples

Title of qualification awarded

PhD in "Design and use of molecules of biotechnological interest"

Dates (from – to)

1998-2003

Name and type of organisation providing education and training	
Principal subjects occupational skills covered	1) 1 ^a Italian school on Molecular Descriptors "Dalla Struttura al Numero", Gargnano del Garda (Italy) 28-30 sept 1998; 2) School of Computational Modeling of Complex systems: Materials, Interfaces, Systems of Biological interest. Perugia (Italy) 28 aug-2 sept 2000; 3) 1 ^o National Seminar for PhD students of Chemistry of Biological Systems: "Modeling e Nuclear Magnetic Resonance: Interactions between Ligands and Macromolecules", Verona (Italy) dal 16-21 July 2001; 4) Training session: "Theoretical Fundaments of Clustering", Focus on research 2003, Sorrento (Italy) 22-23 oct 2003

Dates 1997

Name and type of organization providing education and training Faculty of Pharmacy, University of Naples "Federico II"

Title of qualification awarded Master Degree in Chemistry and Pharmaceutical Technology (110/110 cum laude)

RESEARCH ACTIVITIES

Research sectors	Computational chemistry, drug design, molecular modeling of biomolecular systems and their complexes, structural determinations of bioactive molecules from NMR data, molecular dynamics simulations of biomolecular systems in water and in membrane environment, in silico screening, target fishing, SAR, chemoinformatics.
Recent Scientific Activities.	Presently, the research activity is mainly focused on the: 1) identification of novel ligands from natural sources for molecular targets of pharmacological interest by docking-based virtual screenings plus molecular dynamics simulations, and/or ligand-based chemoinformatic approaches, 2) repositioning of already approved drugs, 3) determination of structure-activity relationships for series of structurally- or functionally-related compounds.
Recent Founded Projects as PI	<i>In silico protein target fishing for naturally occurring acid derivatives and hydroxylated metabolites of plant cannabinoids and experimental validation by in vitro assay.</i> Financed by GW Pharma (UK) (2015-2021). Prin 2017 "Bioactivity-directed exploration of the phytocannabinoid chemical space"
Referee for international peer reviewed Journals.	Bioorganic Chemistry, Journal of Enzyme Inhibition and Medicinal Chemistry, Journal of Medicinal Chemistry, Antioxidants, Cannabis and Cannabinoid Research, Biomolecules, ACS Medicinal Chemistry Letters, Marine Drugs.
Editorial duties	Guest Editor of Special Issue "Molecular Docking in Marine Drug Discovery & Design" (2019) and "Identification and Characterization of Marine Natural Compounds Targeting Nuclear, Ionotropic, or Metabotropic Receptors" (2021) in Marine Drugs Journal; Editorial board member of Marine Drugs Journal in 2020; Guest editor of the Research Topic "Small molecules Targeting Transmembrane Receptors and Ion Channels in Drug Discovery" (2021) in Frontiers in Molecular Biosciences
Scientific Production (2021)	Author of > 60 full papers in ISI Journals, 5 chapters in international books and 1 international patent. Scopus H-index 21/ google scholar H-index 24, i10-index 36 (query date 2021-10-05)