

CURRICULUM VITAE



PERSONAL INFORMATION

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| Name and Surname | MARIANGELA AGAMENNONE |
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| Scopus ID | 6506766137 |
| Google Scholar | https://scholar.google.com/citations?user=V0dqytwAAAAJ&hl=it |

PRESENT POSITION

December 2022 - present

Associate Professor in Medicinal Chemistry (SSD CHEM07-A, SC 03/D1)

Department of Pharmacy

University "G. d'Annunzio" of Chieti-Pescara - Italy

Prof. Agamennone has more than 20 years of experience managing a research lab focused on the application of computational methods (molecular mechanics, docking, pharmacophore modeling, chemoinformatics, (3D-)QSAR, and molecular dynamics) to support the drug design and discovery process.

The main studied targets are: MMPs and other zinc proteases, protein-protein interactions (PD-1/PD-L1 and p53/MDM2), viral hemagglutinin, and α - and β -galactosidases.

Principal research topics focus on cancer, lysosomal storage diseases, anti-influenza drugs, cancer immunotherapy.

WORK EXPERIENCES

March 2017

Awarded the **National Scientific Qualification (ASN 2016)** for the position of Associate Professor, SC 03/D1, SSD CHIM/08.

February 2005 – November 2022

Assistant Professor of Medicinal Chemistry (SSD CHIM/08, SC 03/D1)

Department of Pharmacy, University "G. d'Annunzio" of Chieti-Pescara - Italy

November 2005- October 2007

Research fellowship

Institution

Siena Biotech SpA, Drug Design Unit, Siena - Italy

Research project

"Identification of new MMPs Inhibitors through X-ray structure of the protein target".

Supervisor

Dr. Alessandro Padova

March 2003 - February 2005

Post-doctoral research fellowship

Institution

Department of Pharmaceutical Sciences, University "G. d'Annunzio" of Chieti, Chieti, Italy

Research project

"Design and synthesis of IRT β -lactamases inhibitors"

Supervisor

Prof. Carlo Gallina

May 2002 - December 2003

Post-doctoral research fellowship

Institution

Dipartimento Farmaco-Chimico-Tecnologico, University of Siena, Siena, Italy

Research project

Computational studies on new boronic acids as IRT β -lactamases inhibitors to be used in the treatment of antibiotic resistance.

Supervisor Prof. Maurizio Botta

July 1999- April 2000

Institution Istituto sperimentale per la Elaiotecnica, Pescara, Italy
Research project Validation of olive oil analysis protocols in collaboration with the IOC (International olive council).
Supervisor Dr. Giovanna Vlahov

EDUCATION

November 2002

Institution University "G. d'Annunzio" of Chieti, Chieti, Italy
Thesis title "MMPs inhibitors that uses the phosphonate, N-hydroxyurea and N-hydroxycarbamate function as Zinc Binding Group: synthesis and biological evaluation".
Supervisor Prof. Carlo Gallina

November 1998

Institution University "G. d'Annunzio" of Chieti, Chieti, Italy
Thesis title "Acid-base and metallic catalysis in the enolization reaction of the 5-acetylpyrazole"
Supervisor Prof. Paolo De Maria
Marks 110/110 cum Laude

July 1993

Institution Liceo Classico Statale "G. d'Annunzio", Pescara, Italy
Marks 60/60

GRANTS AND CONTRACTS

September 2025 – June 2026

Funding Program **MITE/MATM Programs**
Project Development of innovative clathrate- and graphene-based materials for hydrogen storage that require low energy input, offer high net energy content, and have a low environmental impact.
Sponsor MASE
Role **Participant**
Grant 2.041.182 €
Duration 9 months

01 August 2024 – 28 February 2025

Funding Program **Research contract**
Project In silico studies of molecules that bind to lysosomal enzymes
Sponsor Galicia Sur Biomedical Foundation, Vigo, Spain
Role **Responsible of the project**
Grant 3.3250 €
Duration 6 months

November 2023 -December 2025

Funding Program **PRIN-PNRR 2022**
Project Investigation of common biochemical pathways, centered around the Amyloid precursor protein (APP), in Alzheimer's Disease and breast cancer models: possible role of Purine Nucleoside Phosphorylase (PNP) – P2022KPMB9_001
Sponsor MIUR
Role **Participant**
Grant 50,000 €
Duration 24 months

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| 17 October 2011 – 17 October 2013 | Funding Program | PRIN 2009 |
| | Project | Modulators of mitochondrial permeability and p53 in the regulation of cell death in cancer cells: identification of new inhibitors of the p53-MDM2/MDMX interaction through virtual screening and the synthesis of low-molecular-weight molecules – 20098SJX4F_005 |
| | Sponsor | MIUR |
| | Role | Participant |
| | Grant | 50,000 € |
| | Duration | 24 mesi |
| 1 novembre 2009 – 31 ottobre 2010 | Funding Program | Applied Research Program 2007 |
| | Project | Study and development of new antiviral drugs against influenza virus A-H1N1 |
| | Sponsor | Ministry of Health |
| | Role | Head of Unit |
| | Grant | 53,000 euros |
| | Duration | 12 months |
| 4 March 2008 – 3 March 2009 | Funding Program | Research contract |
| | Project | “Identification of small molecules inhibitors of protein-protein interactions to be used in the treatment of CNS’ tumours” inserted in the European Project DePPICT no. LSHM-CT-2007-03783. |
| | Sponsor | Siena Biotech SpA, Siena, Italy |
| | Role | Responsible of the project |
| | Grant | 7,500 € |
| | Duration | 12 months |

TEACHING ACTIVITY

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| October 2022 - present | Lecturer and head of the examination board of Advanced Methodologies in Medicinal Chemistry (6 CFU) in the course of Chemistry and Pharmaceutical Technology, University “G. d’Annunzio” of Chieti, Italy. |
| March 2022 - present | Lecturer and head of the examination board of Analisi dei Medicinali (qualitative inorganic analysis) (6 CFU) in the course of Chemistry and Pharmaceutical Technology, University “G. d’Annunzio” of Chieti, Italy. |
| March 2005 - 2021 | Lecturer and head of the examination board of Analisi dei Medicinali (qualitative inorganic analysis) (10 CFU) in the course of Chemistry and Pharmaceutical Technology, University “G. d’Annunzio” of Chieti, Italy. |
| October 2016 – January 2024 | Lecturer and head of the examination board of Progettazione e sviluppo dei farmaci (Drug design and development) (3 CFU) in the course of Chemistry and Pharmaceutical Technology, University “G. d’Annunzio” of Chieti, Italy. The course is organized in 16 hours of lessons and 12 hours of computer practice. |
| AA 2019-2020 | Teacher in the II level University Master Course in “Management of the territorial Pharmacy” |
| March 2005 - present | Supervisor of almost 30 Master degree Thesis for the courses of Pharmacy and Chemistry and Pharmaceutical Technology, University “G. d’Annunzio” of Chieti, Italy. |
| 10 February 2022 and 3 April 2023 | Lessons for the students of the Master of Science ‘Food Chemistry’ at the Technical University of Munich following the course of Introduction to Chemoinformatics and Bioinformatics for Food Scientists” (WZ1330) |
| 21 and 23 June 2022 | Lessons given during the visit of the University of Porto in the Erasmus program Staff Mobility for Teaching |

14 October 2022 Lessons for the students of the PhD School of Biomolecular and Pharmaceutical Sciences, Università "G. d'Annunzio" di Chieti, Italy.

2007 - present Organization of **seminars** for the master students and for the PhD students of the course of Biomolecular and pharmaceutical Sciences. Invited speakers:

2007 Franco Lombardo, Novartis, Cambridge, MA, USA

2009 Graeme Robertson, SienaBiotech, Siena, Italy

2012 Andreas Heine, Philipps-Universität Marburg, Germany

2013 Andrea Beccari, Dompè, L'Aquila, Italy

2014 Elena Petricci, Università di Siena, Siena, Italy

2017 Alessandro Padova, Fondazione RiMed, Palermo, Italy

2019 Andrea Altieri, Edasa scientific, Mosca, Russia

2019 Alexander Kurkin, Lomonosov State University, Mosca, Russia

2022 Pedro Besada, University of Vigo, Vigo, Spain

2022 Saida Ortolano, Instituto de Investigación Sanitaria Galicia Sur, Vigo, Spain

2025 Mariangela Sodano, Axxam, Naples, Italy

2025 Antonella Ciancetta, University of Ferrara, Italy

2025 Maria Elizabeth Tiritan, University of Porto, Portugal

MENTORING ACTIVITY

13 January – 31 March 2025
Project title Dr. Claudia Pinto, PhD student from the University of Porto, **ERASMUM+ Traineeship** program
Nature-inspired chiral flavonoids as potential antitumour agents: a mindset-shifting strategy to achieve eco-friendly drugs

May - July 2023
Project title Dr. Noelia Carmona Zafra, PhD student, University of Madrid, **ERASMUM+ Traineeship** program
Molecular docking studies of curcumin analogues.

September 2022 – February 2023
Project title Shorug Naji, undergraduate student, Anadolu University, Turkey, **ERASMUS + Program**
In silico studies of COX-2 inhibitors (Master Thesis)

July 2022 – August 2022
Project title Prof. Pedro Besada Pereira, University of Vigo, Spain. **Visiting Researcher** of the University of Chieti.
Computational studies of β -galactosidase ligands

April 2014 – February 2015
Project title Tutor of the **Research fellowship** granted by Regione Abruzzo (P.O.F.S.E. 2007-2013)
New strategies for diagnostic, therapeutic and clinical care infection and immunity.

December 2012 – November 2013
Project title Tutor of the **Research fellowship** granted by MIUR
Identification and study of new MMP inhibitors through computational studies.

March 2010 – February 2011
Project title Tutor of the **Research fellowship** granted by the project "Study and development of new antiviral drugs against influenza virus A-H1N1"
Computational approaches for the identification of new molecules blocking the hemagglutinin with potential anti-influenza activity.

January 2009 – December 2011
Project title Tutor of a **European PhD** in Pharmaceutical Sciences, XXIV cycle
Computational and crystallographic studies of zinc-containing enzyme inhibition.
The thesis work was awarded the Bernardo Nobile Prize for PhD Thesis exploiting patent data.

INSTITUTIONAL ACTIVITIES

May 2026 - present Referent for the IRIS database management of the Pharmacy Department.

May 2025 - present

Referent for the Placement service for the course of Chemistry and Pharmaceutical Technology

AA 2019-2020

Board member of the II level University Master Course in "Management of the territorial Pharmacy"

June 2017 – December 2019

Board member for the assignment of mentoring grants for undergraduate students.

October 2008 – September 2009

Member of the PhD program teaching committee (code DOT0353348).

INTERNATIONAL COLLABORATIONS

Prof. A. Di Pizio, Leibniz-Institute for Food Systems Biology at the Technical University of Munich, Freising, Germany.

Prof. A. V. Kurkin, Chemistry Department, Lomonosov Moscow State University, Moscow, Russia.

Prof. J. C. Menendez, Unidad de Química Organica y Farmaceutica, Departamento de Química en Ciencias Farmaceuticas, Facultad de Farmacia, Universidad Complutense, Madrid, Spain

Dr. S. Ortolano, Instituto de Investigación Sanitaria Galicia Sur (IIS Galicia Sur), Vigo, Spain.

Prof. Lukasz Skalniak, Jagiellonian University, Krakow, Poland

Dr. M. Tauro, Departments of Tumor Biology, Moffitt Cancer Center and Research Institute, Tampa, FL, USA.

Prof. M. E. Tiritan, University of Porto, Porto, Portugal.

NATIONAL COLLABORATIONS

Prof.ssa M. Sala Dipartimento di Farmacia, Università di Salerno

Prof. S. Carradori Dipartimento di Farmacia, Università "G. d'Annunzio" di Chieti-Pescara

Dr. F. Superti, National Centre for Innovative Technologies in Public Health, National Institute of Health, Roma

Prof. M. Ronci Dip. di Scienze Mediche Orali e Biotecnologiche, Università "G. d'Annunzio" di Chieti-Pescara

Prof. C. Supuran, Dipartimento di Neuroscienze, Area del Farmaco e Salute del Bambino, Università degli studi di Firenze

Prof. Paolo Tortorella, Dipartimento di Farmacia-Scienze del Farmaco, Università degli Studi "Aldo Moro" di Bari

REVIEWING ACTIVITY

February 2017

External reviewer of the **PhD thesis** of Dr. Alessia Caradonna University of Bari

April 2018

External reviewer for the **research project** PRELUDIUM of National Science Centre Poland

September 2021

External reviewer for **VQR2015-19**

- March 2022** External reviewer for the research project **FARE 2020**
- March 2023** External reviewer of the **PhD thesis** of Dr. Alessandra Riccio University of Perugia
- 15 May 2026** Member of the Doctoral Program Committee in Research Methods in Science and Technology – XXXVIII Cohort - Candidate: David Sotillo Núñez

EDITORIAL ACTIVITY

- 2005-present** Reviewer for several **journals** such as: Journal of Medicinal Chemistry, European Journal of Medicinal Chemistry, Bioorganic and Medicinal Chemistry Letters, Biomolecules, Molecules, Pharmaceuticals, International Journal of Molecular Sciences, New Journal of Chemistry, Future Medicinal Chemistry, Chemmedchem, Drug Research, Scientific Reports, Journal of Computer-Aided Molecular Design, Bioorganic and Medicinal Chemistry, MedChemCom.
- October 2021 - present** **Section Editor** of “In silico Drug Design” section, journal “Letters in Drug Design and Discovery” (Bentham). <https://benthamscience.com/journals/letters-in-drug-design-and-discovery/editorial-board/>
- November 2021 – June 2023** **Guest Editor** of the special issue “Computational Methods in the Design of Anticancer Drugs”, journal Pharmaceuticals (MDPI). https://www.mdpi.com/journal/pharmaceuticals/special_issues/computational_anticancer

PROFESSIONAL MEMBERSHIP

Member of the Italian Chemical Society since 1999

AWARDS AND COVER

- 2026** **Seal of Excellence** for the proposal n. 101278231 — INOUT “Design and formulation of novel tool-based stealth liposomes targeted EGFR, loaded with apigenin-derivatives, fighting breast cancer” submitted under the Horizon Europe Marie Skłodowska-Curie Actions call HORIZON-MSCA-2024-PF-01-01 — MSCA Postdoctoral Fellowships 2025
- 2025** **Seal of Excellence** for the proposal n. 101212131 — INOUT “Design and formulation of novel tool-based stealth liposomes targeted EGFR, loaded with apigenin-derivatives, fighting breast cancer” submitted under the Horizon Europe Marie Skłodowska-Curie Actions call HORIZON-MSCA-2024-PF-01-01 — MSCA Postdoctoral Fellowships 2024
- 2021** The chapter published on Methods in cell biology was awarded the **cover** of the 166th volume of the book series entitled Biomolecular interactions part A.. <https://www.elsevier.com/books/biomolecular-interactions-part-a/shukla/978-0-12-823351-1>
- 2013** The article published on Chemmedchem entitled “Probing the S1’ Site for the Identification of Non-Zinc-Binding MMP-2 Inhibitors” (ChemMedChem, 2013, 8, 1475 – 1482) was awarded **Very Important Paper** (VIP) and Cover picture
- 2011** The article published on Chemmedchem entitled “Biphenyl Sulfonylamino Methyl Bisphosphonic Acids as Inhibitors of Matrix Metalloproteinases and Bone Resorption” (ChemMedChem, 6, 2011, 1258-1268) was awarded **Very Important Paper** (VIP) and Cover picture
- July 2002** XXII Advanced course in Pharmaceutical Chemistry and National seminar for Ph.D students E. Duranti, Urbino. Poster first classified and selected for oral communication.

CONGRESS ORGANIZATION

- 21-25 September 2024** Member of the Organizing Committee of the Molecular Electronic Structure (MES) conference, Pescara, Italy.
- 17-20 September 2023** Member of the Organizing Committee of the XXVIII National Meeting in Medicinal Chemistry, Chieti, Italy.
- 16-20 September 2007** Member of the Organizing Committee of the XVIII National Congress of Medicinal Chemistry Chieti, Italy.

ORAL COMMUNICATIONS AND SEMINARS

- 7 April 2026** Invited speaker in the Seminar Program of the Instituto de Investigación Sanitaria Galicia Sur (IIS Galicia Sur), Vigo, Spain.
Title In Silico Drug Discovery: Accelerating the Search for Bioactive Compounds Through Computational Methods (seminar)
- 22-26 February 2022** 4th International Conference on PharmScience Research & Development. San Francisco, USA. Hybrid
Title Fighting Flu: biological and computational profile of new small molecules targeting hemagglutinin (oral presentation).
- 1-30 November 2021** 7th International Electronic Conference on Medicinal Chemistry,
Title Unraveling the binding mechanism of macrocycle peptides to PD-L1 through computational approaches (oral presentation)
- 28-29 March 2019** IV Computationally Driven Drug Discovery, Rome, Italy.
Title Drugging the undruggable: the prion protein as a case study of aggregating proteins (oral presentation)
- 6-7 June 2014** X National Congress of the Italian Pharmaceutical Microbiology Society, Chieti, Italy
Title Identificazione e studio di nuovi agenti antinfluenzali ad ampio spettro (oral presentation)
- 04-06 February 2013** II Computationally Driven Drug Discovery, Genova, Italy
Title Combined virtual screening protocol for the identification of novel protein-protein interaction inhibitors (oral presentation)
- 21-23 November 2011** I Computationally Driven Drug Discovery. L'Aquila, Italy.
Title Virtual screening approaches for the identification of novel non-zinc-binding MMP inhibitors (oral presentation)
- 1 December 2009** Department of Chemistry, University of Alabama at Birmingham, USA.
Title Fragment-based drug discovery: targeting the S100B-p53 interaction (seminar)
- 13-14 February 2009** III Meeting New Perspectives in Medicinal Chemistry. Castelvecchio Pascoli (LU), Italy.
Title Fragment-based discovery of S100B inhibitors combining computational and biophysical approaches (oral presentation)
- 01-05 July 2002** XXII Advanced course in Pharmaceutical Chemistry and National seminar for Ph.D. Urbino, Italy.
Title Matrix metalloproteinases inhibitors, synthesis and biological evaluation (oral presentation)

PATENTS

European patent number **EP 2780365 B1**

Title *Lactoferrin derived peptides for use as broad- spectrum inhibitors of influenza virus infection*
Applicants Istituto Superiore di Sanità, University "G. d'Annunzio" of Chieti
Inventors Superti F. E.D., Agamennone M., Ammendolia M.G., Pietrantonì A., Lanutti F.
Deposition date 16.11.2012

Italian Patent No **000140832**

Peptidi della Lattoferrina per l'uso come inibitori ad ampio spettro dell'infezione da virus dell'influenza

Applicants Istituto Superiore di Sanità, University "G. d'Annunzio" of Chieti
Inventors Superti F. E.D., Agamennone M., Ammendolia M.G., Pietrantonì A., Lanutti F.
Deposition date 16.11.2011

BIBLIOMETRY

| | |
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| Scopus | by May 25th 2026 |
| Articles | 59 |
| Citations | 1104 |
| H-index | 21 |

PUBLICATIONS

Scopus <https://www.scopus.com/authid/detail.uri?authorId=6506766137>

Google Scholar <https://scholar.google.com/citations?user=V0dqytwAAAAJ&hl=it>