





PERSONAL INFORMATION

Antonio Lupia




 [Redacted], Italy (IT)

 +39 070/675-6839 (studio); 6812 (lab)  [Redacted]

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 <https://orcid.org/0000-0003-0870-2376>

Sex Male | [Redacted] | Nationality Italian

WORK EXPERIENCE

01-03-2023 – To Date

Researcher (RTDa)

“Computer Aided Drug Design of Cagliari (CADDLab)”

University of Cagliari
Cittadella Universitaria di Monserrato
09042 Cagliari (CA)
Department of Life and Environmental Sciences (DISVA)
SSD CHEM-07/A Chimica farmaceutica (ex CHIM/08)

Current project

INF-ACT Project

“ONE HEALTH BASIC AND TRANSLATIONAL RESEARCH ACTIONS ADDRESSING UNMET NEEDS ON EMERGING INFECTIOUS DISEASES - CUP F53C22000720007 – CODICE MUR: PE0000007 - CODICE SELEZIONE”;
THE SCIENTIFIC INTERESTS CONCERN THE APPLICATION OF IN SILICO COMPUTATIONAL METHODS, INCLUDING PHARMACOPHORE, MOLECULAR DOCKING, AND MOLECULAR DYNAMICS, AS WELL AS A GREAT INTEREST IN THE STUDY AND APPLICATION OF PROCESSES BASED ON MACHINE LEARNING (ML) TO INVESTIGATE THE DRUG-RECEPTOR INTERACTIONS, DESIGN AND LEAD-OPTIMISATION OF POTENTIAL DRUGS.
THE MAIN RESEARCH TOPIC IS FOCUSED ON THE FLAVIVIRIDAE FAMILY (DENV 1-2-3-4), ZIKA, WNV, YFV, AND IN PARTICULAR ON BOTH HELICASE/PROTEASE COMPLEXES, WHICH HAVE BEEN ESTABLISHED AS A VALUABLE TARGET FOR DRUG DESIGN TO TREAT ALL FLAVIVIRUS INFECTIONS

Scientific Supervisor *Prof Elias Maccioni*

01-10-2022 al 28-02-2023

Postdoctoral Research

University of Naples “Federico II”
Via Domenico Montesano, 49 – 80131, Naples (NA), Italy
SSD CHEM-07/A

Project

“Rational design with computational methods and chemical synthesis of bile acids and derivatives as potential agonists of the ACE2 enzyme and inhibitors of the interaction between ACE2 and the Spike protein of SARS-CoV-2”

Scientific Supervisor *Prof Bruno Catalanotti*

01-10-2021 al 30-09-2022

Postdoctoral Research

University of Naples “Federico II”
Via Domenico Montesano, 49 - 8013, Naples (NA), Italy

SSD CHEM-07/A
 Project "Intestinal microbiota, bile acids activated receptors and metabolism: development of novel therapeutic targets in the treatment of steato-hepatitis (NASH)"
 Scientific Supervisor *Prof Vittorio Limongelli*

from 01-08-2019 to 31-03-2021 **Researcher and co-founder of the Net4Science academic spinoff and start-up**
 Net4Science srl (N4S), academic spinoff
 c/o University "Magna Græcia" of Catanzaro
 Campus Universitario "S. Venuta", Viale Europa, 88100, Catanzaro (CZ), Italy
 Scientific Supervisor *Prof Stefano Alcaro*
 CEO *Prof Francesco Ortuso*

EDUCATION AND TRAINING

from 26-06-2024 to 26-06-2035 **Abilitazione Scientifica Nazionale (ASN)**
 Settore Concorsuale 03/D1 - II Fascia - Primo Quadrimestre

from 13-02-2024 to 25-02-2024 **Visiting Researcher (Fellowship)**
 Freie University of Berlin (Germany)
 Scientific Supervisor *Prof. Gerhard Wolber*

from 22-01-2024 to 26-01-2024 **Visiting Researcher (Fellowship)**
 University of Porto (Portugal)
 Scientific Supervisor *Prof. Maria Fernanda Martins Borges*

from 05-11-2021 to 16-12-2023 **Master Universitario di II livello – Luiss Business School**
 Master in Management della Filiera della Salute
 "Major in Sperimentazione Clinica: aspetti regolatori, gestionali, operativi"
 c/o Luiss Business School

- Institutional structures and financing systems
- Legislative and regulatory aspects
- Planning a clinical study
- The authorization process for a clinical study
- Management and conduct of clinical studies
- Monitoring and control of clinical trials
- Analysis of the results

Scientific Supervisor *Dott. Gianfranco De Feo, Dirigente della Direzione Scientifica I.N.T. Fondazione G. Pascale (Napoli)*
 CEO *Dott. Fabrizio Galliccia, Dirigente di I livello delle professionalità sanitarie – Ispettore Senior GCP presso AIFA*

from 05-11-2015 to 05-04-2019 **PhD thesis defense and final exam – Università "Magna Græcia" di Catanzaro**
 PhD in Life Science
 Title "Molecular modelling of epitopes recognised by neoplastic B-cells in Chronic Lymphocytic Leukemia (CLL)"

from 31-01-2018 to 31-07-2018 **Visiting PhD Student**
 Istituto Oncologico di Ricerca (IOR), Via Vincenzo Vela 6, 6500, Bellinzona, (CH)
 Scientific Supervisor(s) *Dr. Francesco Bertoni*
Dr. Eugenio Gaudio

22-10-2015 Master Degree in Pharmacy



ACCADEMIC ACTIVITIES

from 01-10-2023 – present

Teacher. Module of protein modeling (CFU 2+1)
MASTER DEGREE COURSE: CELLULAR AND MOLECULAR BIOLOGY Curriculum: Curriculum Advanced cellular studies (coorte: 2023)
[BF/0034/EN] BIOINFORMATICS

from 13-02-2024 to 25-02-2024

Erasmus+ Staff Mobility for Teaching (MOSTA)
Freie University of Berlin (Germany)

from 22-01-2024 to 26-01-2024

Visiting Scientist and teaching (16 hours)
Porto University, Facoltà di Scienze, Dipartimento di Chimica e Biochimica

28-10-2023

Drug Discovery 2030:
A Roadmap for a New Decade Committee Erasmus+ Blended Intensive Programme (BIP) – (2 hours)

from 18-12-2018 – present

Spinoff co-founder
Net4Science srl (N4S), spinoff accademico d/o Università "Magna Græcia" di Catanzaro, Campus Universitario "S. Venuta", Viale Europa, 88100, Catanzaro
Net4Science
Codice Fiscale/P.IVA: 0366606079
Registro delle Imprese di CATANZARO (IT)
Data atto di costituzione: 18-12-2018
www.net4science.com

AWARDS

15-06-2019

Paul Ehrlich Euro-PhD award.

05-12-2020

ANGI Award 2020 – "Associazione Nazionale Giovani Innovatori".

Membership

2025

Scientific Committee "AMYC-BIOMED 2025" @Palermo, 23-25 June 2025.

2024

Organizing Committee "NGC24 - Next Generation Chemists – La Parola ai Giovani 2024" @Sassari, 3-4 October 2024.
SCI Sezione Sardegna

2021

Organizing Committee "Paul Ehrlich (PE) Euro-PhD Network virtual meeting #PEVM2021" 26-28 July, 2021

2020

Member of Società Chimica Italiana (SCI) Divisione di Chimica Farmaceutica.
Tessera SCI: 23478

2019

Organizing Committee "Paul Ehrlich Euro-PhD Network & MuTalig COST -Action meeting 2019", @Catanzaro (Italy), 13-15 June, 2019

PERSONAL SKILLS

Mother tongue(s)	Italian				
Other language(s)	UNDERSTANDING		SPEAKING		WRITING
ENGLISH	Listening	Reading	Spoken interaction	Spoken production	
Replace with language	C1	C1	C1	C1	C1

Skill Highlights

- Knowledge of computational techniques in the Drug Discovery process
- Excellent command of molecular modelling software (Schrödinger suite, LigandScout, AMBER, Autodock, FLAP, KNIME)
- Good knowledge of programming languages (Python, PHP, JavaScript, and HTML editing)
- Excellent skills with Adobe Illustrator, CyberLink Power Director and others related to Photo/Video/Music editing
- Excellent command of Microsoft Windows OS, Linux OS and Mac OS.

Soft Skill

- Professionalism, coherence, and respect
- Creativity and attention to detail
- High flexibility and adaptation in a new context
- High problem-solving skills, motivation, and goal bearings

Driving licence

- B

ADDITIONAL INFORMATION

[ResearchGate](#)

[LinkedIn](#)

[ORCID](#)

[List of Publications](#) (or via [SCOPUS](#))



Short CV

Antonio Lupia

University of Cagliari – Department of Life and Environmental Sciences

Antonio Lupia graduated in Pharmacy at the University of "Magna Græcia" of Catanzaro in 2015. He received his Ph.D. in Life Sciences at the University of "Magna Græcia" of Catanzaro in 2019, defending a thesis entitled "Molecular modelling of epitopes recognised by neoplastic B-cells in Chronic Lymphocytic Leukemia (CLL)" and also receiving the Paul Ehrlich Euro-PhD award. During his young career, Antonio worked in the Molecular Design Lab group at the Freie University of Berlin, in Gerhard Wolber's Lab, and at the Institute of Oncology Research (IOR) of Bellinzona, Switzerland. After two postdoctoral fellowships (2021 to 2023) in Computational Chemistry at the University Federico II of Naples, he currently joined the Faculty of Biology and Pharmacy of Cagliari as researcher (RTDA) working in the Computer Aided Drug Design (CADD) Group of the Department of Life and Environmental Sciences.

The scientific interests concern the application of computational methods, including Pharmacophore, Molecular Docking, 3D-QSAR, Molecular Dynamics and Virtual Screening techniques, as well as a great interest in the study and application of processes based on Machine Learning (ML) to investigate the drug-receptor interactions, design, and lead-optimisation of potential drugs. Antonio has collaborated with prestigious international research teams in research-related projects and as part of the Scientific/Organizer Committee of national/international meetings. Finally, he is a co-founder of the Net4Science academic spinoff.

Recent Publications (up to 10)

1. Coricello, A., Nardone, A.J., Lupia, A. et al. 3D variability analysis reveals a hidden conformational change controlling ammonia transport in human asparagine synthetase. *Nat Commun* 15, 10538 (2024).
2. Finamore, et all.; Exploring Boswellia serrata Triterpenes: A New Frontier in Leukemia Inhibitory Factor Receptor Modulation. *ACS Omega*, Pages 22269 - 222843 June 2025.
3. The leukemia inhibitory factor regulates fibroblast growth factor receptor 4 transcription in gastric cancer. Di Giorgio, C., Bellini, R., Lupia, A., ...Zampella, A., Fiorucci, S. *Cellular Oncology*, 2024, 47(2), pp. 695–710.
4. Exploring the DNA2-PNA heterotriplex formation in targeting the Bcl-2 gene promoter: A structural insight by physico-chemical and microsecond-scale MD investigation. Falanga, A.P., Lupia, A., Tripodi, L., ...Oliviero, G., Borbone, N. *Heliyon*, 2024, 10(3), e24599.
5. Molecular and Structural Aspects of Clinically Relevant Mutations of SARS-CoV-2 RNA-Dependent RNA Polymerase in Remdesivir-Treated Patients. Gratteri, C., Ambrosio, F.A., Lupia, A., ...Artese, A., Alcaro, S. *Pharmaceuticals*, 2023, 16(8), 1143.
6. Development of Cyclic Peptides Targeting the Epidermal Growth Factor Receptor in Mesenchymal Triple-Negative Breast Cancer Subtype. Nisticò, N., Aloisio, A., Lupia, A., ...Quinto, I., Iaccino, E. *Cells*, 2023, 12(7), 1078.
7. Discovery of BAR502, as potent steroidal antagonist of leukemia inhibitory factor receptor for the treatment of pancreatic adenocarcinoma. Di Giorgio, C., Bellini, R., Lupia, A., ...Zampella, A., Fiorucci, S. *Frontiers in Oncology*, 2023, 13, 1140730 .
8. Molecular Basis for Non-Covalent, Non-Competitive FAAH Inhibition. Morgillo, C.M., Lupia, A., Deplano, A., ...Moraca, F., Catalanotti, B. *International Journal of Molecular Sciences*, 2022, 23(24), 15502.
9. Repositioning Mifepristone as a Leukaemia Inhibitory Factor Receptor Antagonist for the Treatment of Pancreatic Adenocarcinoma. Di Giorgio, C., Lupia, A., Marchianò, S., ...Zampella, A., Fiorucci, S. *Cells*, 2022, 11(21), 3482.
10. Ligand-based drug repurposing strategy identified SARS-CoV-2 RNA G-quadruplex binders. Moraca, F., Marzano, S., D'Amico, F., ...Pagano, B., Amato, J. *Chemical Communications*, 2022, 58(85), pp. 11913–11916.

