europass Curriculum vitae

PERSONAL INFORMATION

Maria Laura De Sciscio

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Date of birth 9 January 1996 | Nationality Italian

RESEARCH EXPERIENCE

04/2024–12/2024 Visiting PhD Student

University College London, London, UK

Supervisor: Franca Fraternali, Project Title: "Molecular dynamics simulations and structural bioinformatics computational investigation of post-translational modifications of proteins leading to misfolded states"

April 2021 – April 2022 Biochemistry Researcher

Campus Bio-Medico, University of Rome, Italy
Supervisor: M. Maccarrone
Project: "Study of new compounds effect on endocannabinoid system activity in human cells"

EDUCATION AND TRAINING

2022–Present PhD in Chemical Science

Sapienza University of Rome, Italy

Supervisor: M. D'Abramo. Thesis Title: "Computational methods for the development and formulation of drugs"

10/2018–03/2021 Master's degree in Chemistry

Bio-Organic curriculum

Alma Mater University, The University of Bologna, Italy

Supervisors: M.Calvaresi, M.Maccarrone. Thesis title: "Comparison of rFAAH and hFAAH: in vitro analysis, computational investigation and possible pharmaceutical implications"

10/2014–05/2018 Bachelor's degree in Chemistry

Sapienza University of Rome, Italy

Supervisor: P. Gentili. Thesis title: "Synthesis of 2-methylpropanoate of 5-hydroxyimino-6-oxohexyl and polymerisation tests"

2014 Italian secondary school diploma: Classical Certificate

Pietro Giannone LIC.CL., BENEVENTO (BN)

PERSONAL SKILLS

Computer skills

- experience with Linux
- experience with Python programming language
- experience with common Molecular Dynamics simulations package (e.g. Gromacs, NAMD)
- experience with common Quantum Chemical calculation software (e.g. Gaussian)
- experience with Microsoft Office programmes

PUBLICATIONS

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[1] Dongjun Guo, **Maria Laura De Sciscio**, Joseph Chi-Fung Ng, and Franca Fraternali. “Modelling the assembly and flexibility of antibody structures”. In: *Current Opinion in Structural Biology* 84 (2024), p. 102757.

[2] Lawanya Natarajan, **Maria Laura De Sciscio**, Alessandro Nicola Nardi, Ashok Sekhar, Alessandra Del Giudice, Marco D’Abramo, and Athi N Naganathan. “A finely balanced order–disorder equilibrium sculpts the folding–binding landscape of an antibiotic sequestering protein”. In: *Proceedings of the National Academy of Sciences* 121.20 (2024), e2318855121.

[3] Antonella Costanzo, Francesca Fata, Ida Freda, **Maria Laura De Sciscio**, Elena Gugole, Giovanni Bulfaro, Matteo Di Renzo, Luca Barbizzi, Cécile Exertier, Giacomo Parisi, et al. “Binding of steroid substrates reveals the key to the productive transition of the cytochrome P450 OleP”. In: *Structure* 32.9 (2024), pp. 1465–1476.

[4] Flavia Catalano, Daniele Santorelli, Alessandra Astegno, Filippo Favretto, Marco D’Abramo, Alessandra Del Giudice, **Maria Laura De Sciscio**, Francesca Troilo, Giorgio Giardina, Adele Di Matteo, et al. “Conformational and dynamic properties of the KH1 domain of FMRP and its fragile X syndrome linked G266E variant”. In: *Biochimica et Biophysica Acta (BBA)-Proteins and Proteomics* 1872.4 (2024), p. 141019.

[5] **Maria Laura De Sciscio**, Alessandro Nicola Nardi, Fabio Centola, Mara Rossi, Enrico Guarnera, and Marco D’Abramo. “Molecular Modeling of the Deamidation Reaction in Solution: A Theoretical–Computational Study”. In: *The Journal of Physical Chemistry B* 127.44 (2023), pp. 9550–9559.

[6] **Maria Laura De Sciscio**, Alessandro Nicola Nardi, Giacomo Parisi, Giovanni Bulfaro, Antonella Costanzo, Elena Gugole, Cécile Exertier, Ida Freda, Carmelinda Savino, Beatrice Vallone, Linda Celeste Montemiglio, and Marco D’Abramo. “Effect of Salts on the Conformational Dynamics of the Cytochrome P450 OleP”. In: *Molecules* 28.2 (Jan. 2023), p. 832.

[7] Emanuele Criscuolo, **Maria Laura De Sciscio**, Angela De Cristofaro, Catalin Nicoara, Mauro Maccarrone, and Filomena Fezza. “Computational and Experimental Drug Repurposing of FDA-Approved Compounds Targeting the Cannabinoid Receptor CB1”. In: *Pharmaceuticals* 16.12 (2023), p. 1678.

[8] **Maria Laura De Sciscio**, Valeria D’Annibale, and Marco D’Abramo. “Theoretical Evaluation of Sulfur-Based Reactions as a Model for Biological Antioxidant Defense”. In: *Int. J. Mol. Sci.* 23.23 (Nov. 2022), p. 14515.

[9] Alessandra Piccirilli, Emanuele Criscuolo, Fabrizia Brisdelli, Paola Sandra Mercuri, Sabrina Cherubini, **Maria Laura De Sciscio**, Mauro Maccarrone, Moreno Galleni, Gianfranco Amicosante, and Mariagrazia Perilli. “Exploring the Role of L10 Loop in New Delhi Metallo-β-lactamase (NDM-1): Kinetic and Dynamic Studies”. In: *Molecules* 26.18 (Sept. 2021), p. 5489.

[10] Emanuele Criscuolo, **Maria Laura De Sciscio**, Filomena Fezza, and Mauro Maccarrone. “In Silico and In Vitro Analysis of Major Cannabis-Derived Compounds as Fatty Acid Amide Hydrolase Inhibitors”. In: *Molecules* 26.1 (Dec. 2020), p. 48.

[11] Filomena Fezza, Emanuele Criscuolo, **Maria Laura De Sciscio**, and Mauro Maccarrone. “Chapter 31 - Fatty acid amide hydrolase, anandamide, and neurological diseases”. In: *Neurobiology and Physiology of the Endocannabinoid System*. Ed. by Vinood B. Patel, Victor R. Preedy, and Colin R. Martin. Academic Press, Jan. 1, 2023, pp. 417–428.

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