Maria Laura **De Sciscio**

Profile Summary

Computational Chemist | Computational Biologist | Machine Learning in Drug Development with over 3+ years of expertise in molecular dynamics, quantum chemical, and QM/MM multiscale simulations. Proficient in data manipulation, statistical analysis, and data visualization. Skilled in data collection, analysis, graphics making, and creating insightful visual reports to facilitate data comprehension.

Contact details

@ marialaura.desciscio@uniroma1.it
✉ Via Ignazio Danti 21, Rome (RM)

Personal information

Year of birth: **1996**
Citizenship: **Italy**
Languages: **English**, **Italian**

Skills

- Linux, Bash, Python, GitHub
- Pandas, Numpy, Scipy, Scikit-learn
- Microsoft Excel, MS Word, MS PowerPoint
- Gromacs, Namd, Gaussian, QChem, Orca
- Pymol, VMD, Chimera, MOE
- Communication and team collaboration

Experience

Adjunct Professor at *Temple University Rome Campus* **01/2025–Present**
◇ Course: General Chemistry I Lab

Research Fellowship at *Sapienza University of Rome, Italy* **02/2025–Present**
◇ Project Title: "Computational-theoretic approaches for the characterization of post-translational modifications". Supervisor: M. D'Abramo.

Visiting PhD Student at *University College London, London, UK.* **04/2024–12/2024**
◇ Project Title: "Molecular dynamics simulations and structural bioinformatics computational investigation of post-translational modifications of proteins leading to misfolded states". Supervisor: F. Fraternali.

Biochemistry Researcher at *Campus Bio-Medico, University of Rome, Italy.* **04/2021 – 04/2022**
◇ Project Title: "Study of new compounds effect on endocannabinoid system activity in human cells". Supervisor: M. Maccarrone.

Education

PhD in Chemical Sciences *from Sapienza University of Rome, Italy.* **2022–Present**
◇ Thesis Title: "Computational methods for the development of biotherapeutics drugs". Supervisor: M. D'Abramo.

Master's degree in Chemistry *Alma Mater Studiorum, The University of Bologna, Italy.* **10/2018–03/2021**
◇ Thesis title: "Comparison of rFAAH and hFAAH: in vitro analysis, computational investigation and possible pharmaceutical implications". Supervisors: M.Calvaresi, M.Maccarrone.

Bachelor's degree in Chemistry *ASapienza University of Rome, Italy.* **10/2014–05/2018**
◇ Thesis title: "Synthesis of 2-methylpropanoate of 5-hydroxyimino-6-oxohexyl and polymerisation tests". Supervisor: P. Gentili.

Conference & Workshops

◇ First Symposium for YouNg Chemists, *Rome, Italy*. Poster **06/2022**
◇ DCTC2022, *Modena, Italy.* Poster **9/2022**
◇ Biophysics@Rome, *CNR, Rome, Italy*. Poster **04/2023**
◇ ISMB Retreat, *Clare College, Cambridge, UK* Poster **07/2023**
◇ 9th CCPBioSim conference, *Leeds University, UK*. Poster Pitch **07/2023**
◇ EuChemS CompChem 2023 "Exploring Molecular Space", *Thessaloniki, Greece*. Poster **08/2023**
◇ CCPBioSim workshop: structural bioinformatics resources and tools for molecular dynamics simulations, *EMBL-EBI, Cambridge*. Trainer **09/2023**
◇ Second Symposium for YouNg Chemists, *Rome, Italy*. Talk **06/2024**
◇ 31th Intl. BIOMOS Symposium on Biomolecular Simulation, *Innsbruck, Austria*. Talk **09/2024**

Maria Laura **De Sciscio**

Pubblications

1. Tuning Antibody Stability and Function by Rational Designs of Framework Mutations. ◇ J. C. F. Ng, A. Chenoweth, **M. L. De Sciscio**, M. Grandits, A. Cheung, T. Chu, A. McCraw, J. Chauhan, Y. Liu, D. Guo, S. Patel, A. Kosmider, D. Iancu, S. N. Karagiannis, and F. Fraternali. **03/2025**
2. Dissecting Methionine Oxidation by Hydrogen Peroxide in Proteins: Thermodynamics, Kinetics, and Susceptibility Descriptors. ◇ **M. L. De Sciscio**, F. Centola, S. Saporiti, and M. D'Abramo. *J. Chem. Inf. Model.* 65(2), 749-761 **01/2025**
3. Corylus Avellana Non-Specific Lipid-Transfer Protein Cor a 8 Is a Moonlighting Enzyme with a New Lipase Activity. ◇ A. Fissore, G. Di Napoli, **M. L. De Sciscio**, V. Santoro, E. Salladini, M. Marengo, S. Oliaro-Bosso, G. Vanzetti, A. Caratti, F. Dal Piaz, F. Piazza, M. Manzoli, G. Genova, A. G. Barbiroli, S. Iametti, F. Fraternali, and S. Adinolfi. **11/2024**
4. Binding of Steroid Substrates Reveals the Key to the Productive Transition of the Cytochrome P450 OleP. ◇ A. Costanzo, F. Fata, I. Freda, **M. L. De Sciscio**, E. Gugole, G. Bulfaro, M. Di Renzo, L. Barbizzi, C. Exertier, G. Parisi, M. D'Abramo, B. Vallone, C. Savino, and L. C. Montemiglio. *Structure* 32(9), Elsevier, 1465–1476.e3. **09/2024**
5. Conformational and Dynamic Properties of the KH1 Domain of FMRP and Its Fragile X Syndrome Linked G266E Variant. ◇ F. Catalano, D. Santorelli, A. Astegno, F. Favretto, M. D'Abramo, A. Del Giudice, **M. L. De Sciscio**, F. Troilo, G. Giardina, A. Di Matteo, and C. Travaglini-Allocatelli. *Biochim. Biophys. Acta - Proteins and Proteomics* 1872(4), p. 141019. **07/2024**
6. A Finely Balanced Order–Disorder Equilibrium Sculpts the Folding–Binding Landscape of an Antibiotic Sequestering Protein. ◇ L. Natarajan, **M. L. De Sciscio**, A. N. Nardi, A. Sekhar, A. Del Giudice, M. D'Abramo, and A. N. Naganathan. *Proc. Natl. Acad. Sci.* 121(20), e2318855121. **05/2024**
7. Modelling the Assembly and Flexibility of Antibody Structures. ◇ D. Guo, **M. L. De Sciscio**, J. C. F. Ng, and F. Fraternali. *Curr. Opin. Struct. Biol.* 84, p. 102757. **02/2024**
8. Molecular Modeling of the Deamidation Reaction in Solution: A Theoretical–Computational Study. ◇ **M. L. De Sciscio**, A. N. Nardi, F. Centola, M. Rossi, E. Guarnera, and M. D'Abramo. *J. Phys. Chem. B* 127(44), American Chemical Society, pp. 9550–9559. **11/2023**
9. Effect of Salts on the Conformational Dynamics of the Cytochrome P450 OleP. **01/2023** ◇ **M. L. De Sciscio**, A. N. Nardi, G. Parisi, G. Bulfaro, A. Costanzo, E. Gugole, C. Exertier, I. Freda, C. Savino, B. Vallone, L. C. Montemiglio, and M. D'Abramo. *Molecules* 28(2), p. 832.
10. Theoretical Evaluation of Sulfur-Based Reactions as a Model for Biological Antioxidant Defense. **01/2022** ◇ **M. L. De Sciscio**, V. D'Annibale, and M. D'Abramo. *Int. J. Mol. Sci.* 23(23), p. 14515.
11. In Silico and In Vitro Analysis of Major Cannabis-Derived Compounds as Fatty Acid Amide Hydrolase Inhibitors. ◇ E. Criscuolo, **M. L. De Sciscio**, F. Fezza, and M. Maccarrone. *Molecules* 26(1), p. 48. **01/2021**
12. Exploring the Role of L10 Loop in New Delhi Metallo–Lactamase (NDM-1): Kinetic and Dynamic Studies. ◇ A. Piccirilli, E. Criscuolo, F. Brisdelli, P. S. Mercuri, S. Cherubini, **M. L. De Sciscio**, M. Maccarrone, M. Galleni, G. Amicosante, and M. Perilli. *Molecules* 26(18), p. 5489. **01/2021**