

PERSONAL INFORMATION

Lorenzo Antonini

📍 Rome

✉ lorenzo.antonini@uniroma1.it

WORK EXPERIENCE

-
- 10/2020–Present **Research Fellow**
Department of Drug Chemistry and Technology, Sapienza University of Rome, Rome (Italy)
- 11/2018–Present **PhD in Pharmaceutical Sciences**
Sapienza University of Rome, Rome (Italy)
- Scientific projects management
 - Molecular Dynamics simulations
 - Free Energy calculations
 - Ligand/structure-based drug design
 - ab initio quantum mechanical calculations
 - QSAR model development
- 02/2018–12/2019 **Scientific Consultant**
AISEA, Milan (Italy)
- Molecular Dynamics simulations
 - Results presentation in group meeting and conference
- 03/2017–12/2019 **Computational Chemistry and Cheminformatics Consultant**
Alchemical Dynamics, Rome (Italy)
- Computational chemistry and cheminformatics consultancy to drug discovery companies
 - Machine learning (QSAR/QSPR)
 - Molecular Dynamics simulations
 - Chemical library analysis and expansion
 - Virtual library design by combinatorial synthesis
 - Ligand/structure-based virtual screening
 - Similarity screening
 - Theoretical support for NMR experiments
- 10/2015–01/2017 **Graduation Internship**
Rome Center for Molecular Design, Department of Chemistry and Technology of Drugs, Sapienza University, Rome (Italy)
- Ab initio quantum mechanical calculations
 - Reaction mechanism investigation
 - Density Functional Theory
 - Car-Parrinello Molecular Dynamics

06/2013–01/2014 Pharmacy Internship
Farmacia Cruciani, Selci (RI) (Italy)

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Supervisor: Prof. Rino Ragno

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Co-supervisor: Prof. Federico Pepi

PERSONAL SKILLS

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Job-related skills

- Scientific computing
- Python Programming Language
- Matlab/Octave Programming Language
- Computing in Unix/Linux Environments
- Management of SQL relational databases

SCIENTIFIC COMMUNICATIONS

Publications

Boriero, D.; Carcereri de Prati, A.; Antonini, L.; Ragno, R.; Sohji, K.; Mariotto, S.; Butturini, E. **The anti-STAT1 polyphenol myricetin inhibits M1 microglia activation and counteracts neuronal death.** *The FEBS Journal* 288 (7), 2020, 2347-2359 <https://doi.org/10.1111/febs.15577>

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Oral Presentations

ATP1A3 wild type and mutated isoforms molecular dynamics simulations in a lipid membrane bilayer. Insights on protein structure and ion interactions. L. Antonini, A. Patsilnakos, R. Ragno. ATP1A3 Symposium in Disease, 3-4/10/2019, Reykjavik, Iceland

Poster

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Towards the construction of a structure-based protocol to select potential ATP1A3 ligands through virtual screening procedures. R. Ragno, A. Patsilnakos, L. Antonini, F. D. Tiziano, R. Piacentini, A. Novelli, C. Grassi, F. Gurrieri. 6th Symposium on ATP1A3 in Disease, 21-22/09/2017, Tachikawa, Tokio, Japan.

Gas phase pentose sugar dehydration mechanism: an ab initio and experimental study. F. Pepi, A. Ricci, S. Garzoli, A. Troiani, C. Salvitti, R. Ragno, A. Patsilnakos, L. Antonini, B. Di Rienzo, P. Giacomello. 65th Conference of Mass Spectrometry and Allied Topics, Indianapolis (USA), 4-8/06/2017.

PRIZES AND AWARDS

Sapienza University Funding for Research 2020

Project title: "STAT3: a molecular dynamics study on gain-of-function and loss-of-function

mutations"

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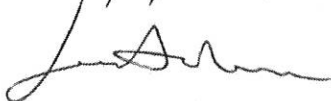
Structure Activity Relationship

11-12/04/2018, Cardiff, UK

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08/09/2017, Sapienza University, Rome, Italy

Rotta 16/08/2021



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