europass Curriculum vitae

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)

EDUCATION AND TRAINING

11/2018–Present PhD in Pharmaceutical Sciences
Sapienza University of Rome, Rome (Italy)
Supervisor: Prof. Rino Ragno

07/2017 Professional qualification of Pharmacist
Sapienza University of Rome, Rome (Italy)

01/2017 Master's Degree in Chemistry and Pharmaceutical Technology
Sapienza University of Rome, Rome (Italy)
Thesis title: "Pentose sugars dehydration in the gas-phase: a theoretical study"
Supervisor: Prof. Rino Ragno
Co-supervisor: Prof. Federico Pepi

PERSONAL SKILLS

Mother tongue(s) Italian

Foreign language(s)

	UNDERSTANDING		SPEAKING		WRITING
	Listening	Reading	Spoken interaction	Spoken production	
English	C1	C1	B2	B2	B2

Levels: A1 and A2: Basic user - B1 and B2: Independent user - C1 and C2: Proficient user
Common European Framework of Reference for Languages - Self-assessment grid

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

Sabatino, M.; Fabiani, M.; Božović, M.; Garzoli, S.; Antonini, L.; Marcocci, M.E.; Palamara, A.T.; De Chiara, G.; Ragno, R. **Experimental Data Based Machine Learning Classification Models with Predictive Ability to Select in Vitro Active Antiviral and Non-Toxic Essential Oils.** *Molecules 2020, 25, 2452.* https://doi.org/10.3390/molecules25102452

Matutino Bastos, T.; Botelho Pereira Soares, M.; Haddad Franco, C.; Alcântara, L.; Antonini, L.; Sabatino, M.; Mautone, N.; Holanda Freitas-Junior, L.; Moraes, C.B.; Ragno, R.; Rotili, D.; Schenkman, S.; Mai, A.; Silvio Moretti, N. **Identification of Inhibitors to *Trypanosoma cruzi***

Sirtuins Based on Compounds Developed to Human Enzymes. *International Journal of Molecular Sciences, 2020, 21, 3659.* https://doi.org/10.3390/molecules25102452

Garzoli, S., Antonini, L., Troiani, A., Salvitti, C., Giacomello, P., Patsilinakos, A., Ragno, R., Pepi, F. **Gas-phase structures and thermochemical properties of protonated 5-HMF isomers.** *International Journal of Mass Spectrometry, 2020, 447, 116237.* https://doi.org/10.1016/j.ijms.2019.116237

Stazi, G., Battistelli, C., Piano, V., Mazzone, R., Marrocco, B., Marchese, S., Louie, S.M., Zwergel, C., Antonini, L., Patsilinakos, A., Ragno, ... Tripodi, M., Nomura, D.K., Mattevi, A., Mai, A., Valente, S. **Development of alkyl glycerone phosphate synthase inhibitors: Structure-activity relationship and effects on ether lipids and epithelial-mesenchymal transition in cancer cells.** *European Journal of Medicinal Chemistry, 2019, 163, 722–735.* https://doi.org/10.1016/j.ejmech.2018.11.050

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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. Patsilinakos, R. Ragno. ATP1A3 Symposium in Disease, 3-4/10/2019, ReykJavik, Iceland

Poster

Machine learning and essential oils: PDIA3 as a case study. L. Antonini, M. Sabatino, E. Proia, F. Sapienza, G. Paglia, M. Eufemi, F. Altieri, R. Ragno. Paul Ehrlich Euro-PhD Network Virtual Meeting 26-28/07/2021.

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Ligand-based virtual screeening of Bcl-2 inhibitors using an ensemble of Machine Learning algorithms. A. Patsilinakos, Y. Carta, M. Sabatino, L. Antonini, R. Ragno. 22nd EuroQSAR 16-20/09/2018, Thessaloniki, Greece.

Gas phase structures and thermochemical parameters of protonated 5-HMF isomers. F. Pepi, S. Garzoli, L.Antonini, G. De Petris, A. Troiani, C. Salvitti, P. Giacomello, R. Ragno, A. Patsilinakos and A. Ricci. XXII International Mass Spectrometry Conference, 26-31/08/2018, Florence, Italy.

Towards the construction of a structure-based protocol to select potential ATP1A3 ligands through virtual screening procedures. R. Ragno, A. Patsilinakos, 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. Patsilinakos, 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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CONFERENCES

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Essential Oils in Medicine, Pharmacy and in the Food Industry
08/09/2017, Sapienza University, Rome, Italy

Roma 16/08/2021

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