LinkedIn page

ELEONORA MENICACCI

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Nationality : Italian

Computational/Medicinal Chemist

Certified Pharmacist of France - Registration as Assistant Pharmacist. RPPS : 2800942791

Excellent Student Award - La Sapienza University of Rome - 05/2016

TECHNICAL SKILLS

- *Molecular modeling and quantum chemistry*
- *Study of the reactivity of inorganic substances (thermo-kinetic and thermodynamic modeling)*
- ***Ligand- and Structure-Based Drug Design, QSAR***
- *Ability to identify physico-chemical descriptors to characterize the chemical reactivity and pharmacological activity of a substance*

INFORMATICS SKILLS

- ***Molecular Dynamics** : GROMACS, Q6*
- *Molecular Modeling: ORCA, **GAUSSIAN**, NWCHEM, Schrödinger Platform, **Maestro***
- ***Docking**: Vina, Autodock4.0, Glide*
- *Molecular Visualisation: VMD, GaussView, GABEDIT, Chimera, JMOL, Avogadro, MGLtools*
- ***Python**,Pandas, NumPy, SciPy, **Scikit-Learn**, **JupyterNotebook**, Bash, HTML, JavaScript*
- *Chemoinformatics tools: **Open Babel**, Pybel, **RDKit**, PubChemPy, JSME, JSMOL*
- *Operative Systems : Linux and Windows*

PROFESSIONAL EXPERIENCE

2023. Postdoctoral Position. ENSTA Paris, UCP (*Unité Chimie et Procédés)*, under the supervision of Prof. Julian Garrec. The project also involves other partners such as IRBA (Institut de recherche biomédicale des armées) and the Institut Polytechnique de Paris. *Melioidosis and antibiotic resistance: modeling and prediction of enzyme mutations. The aim is to study, at the molecular level, a key mechanism of antibiotic resistance in melioidosis. The study will allow the development of a predictive tool for the appearance of this type of resistance.*

2021 – 2022. Assistant Pharmacist. Pharmacie du marché, 93120, La Courneuve. *Dispensation of medicines and offering information to patients regarding dosage, side effects, drug interaction. Maintenance of patient profiles, inventories, pharmacy files, and other records. Reduction pharmacy waste by enacting better protocols for inventory and storage. Run screening programs for blood pressure. Order and control stock.*

2018. Teaching Experience, University of Paris Descartes, « Faculté des sciences fondamentales et biomédicales », *« Licence 2 Séparative methods », 14 hours.*

EDUCATION

2016 – 2019. PhD in Computational Chemistry. Chimie ParisTech, ENSCP, *under the direction of Prof. Carlo Adamo and Patricia Rotureau. Thesis funded by **INERIS** - National Institute for Industrial Environment and Risks - Theoretical study of the thermal decomposition of ammonium nitrate (AN) in presence of additives and contaminants using a **molecular modeling** approach. Simulation and **prediction of the reactivity** of AN in contact with different substances to understand its reactivity, the key steps of the reactions and the resulting energy profile, with the help of **density functional theory** level of calculation. Prevention of industrial chemical risk associated with the utilization, transport and storage of AN.*

2009 – 2015. Diploma in Medicinal Chemistry. La Sapienza University of Rome - *Final Score: **110/110 Cum Laude***

2013 – 2015. Internship in Chemoinformatics. La Sapienza University - Rome Center of Molecular Design (RCMD) – Rome. *Under the supervision of Prof. Rino Ragno. Development of a **database** of **natural molecules with pharmacological activity**, using **python** programming language, **django** framework and many others **chemoinformatics tools**.*

CERTIFICATION

10th-14th June 2024. Spring School Structure-based Computer–aided Drug Design at SIB (Swiss Institute of Bioinformatics).

February 2024. IBM Data Science Coursera certificate (In progress). *Data Science, Big Data, Python Programming, Github, Machine Learning, Deep Learning, Methodology, SQL, Rstudio, Data Mining, Jupyter notebooks*

Avril 2020. Schrödinger Certification Online Course: Introduction to Molecular Modeling in Drug Discovery.

March 2019. Spring School on Computational Chemistry CSC IT Center for Science - Helsinki – Finland. *Classical molecular dynamics, **electronic structure theory**, **machine learning applied to chemistry**. Software used: GROMACS, ORCA, GABEDIT, NWCHEM, JMOL.*

SOFT SKILLS

- ***Rigor, proactivity, curiosity***
- *Ability to identify priorities, get organized and keep commitments*
- *Balance between **team and individual work***
- *Analyze the causes of a problem to solve it*

LANGUAGES

- ***Italian**: Mother Tongue*
- ***French**: Fluent*
- ***English**: Fluent*

INTERESTS

- *Yoga, reading, cooking*

CONFERENCES and CONGRESSES

- *Les JTMS18. Theory, Modeling and Simulation Days. Paris, May 2018.* ***Poster***
- *RCTF. Meeting of French-Speaking Theoretical Chemists. Toulouse, October 2018.* ***Poster***
- *Loss Prevention 2019. Delft, Netherlands, June 2019.* ***Oral Presentation***
- *« Opération CIEDS 2023 ». IPP, June 2023.* ***Poster***

LIST OF PUBLICATIONS

Only non-confidential work

- *Menicacci, E.; Rotureau, P.; Fayet, G.; Adamo, C. Investigation of Ammonium Nitrate Contaminants Based on Computational Chemistry Approach. Chem. Eng. Trans.* ***2019****, 77 (November 2018), 325–330. https://doi.org/10.3303/CET1977055.*

- *Menicacci, E.; Rotureau, P.; Fayet, G.; Adamo, C. Toward the Mechanistic Understanding of the Additives' Role on Ammonium Nitrate Decomposition: Calcium Carbonate and Calcium Sulfate as Case Studies. ACS Omega* ***2020****, 5 (10), 5034–5040. https://doi.org/10.1021/acsomega.9b03964.*

- *Thesis Manuscript. Eleonora Menicacci. Étude théorique de la décomposition thermique du nitrate d'ammonium en présence d'additifs et de contaminants. Chimie théorique et/ou physique. Université Paris sciences et lettres,* ***2019****. Français. NNT: 2019PSLEC026. tel-03143138.* Click here to download my manuscript!