Martí **Municoy Terol**

✉ martimunicoy@gmail.com | martimunicoy | martimunicoy

Education

M.Sc. in Modelling for Science and Engineering   *Barcelona, Spain*

Universitat Autònoma de Barcelona   *2017 - 2018*

- Specialization in Data Science

**B.Sc. in Chemistry**   *Barcelona, Spain*

Universitat Autònoma de Barcelona   *2011 - 2017*

B.Sc. in Physics   *Barcelona, Spain*

Universitat Autònoma de Barcelona   *2011 - 2017*

Programming skills

Python, C and C++, HTML5 and CSS, SQL, GNU Bash, LaTeX, GitHub

Scientific software
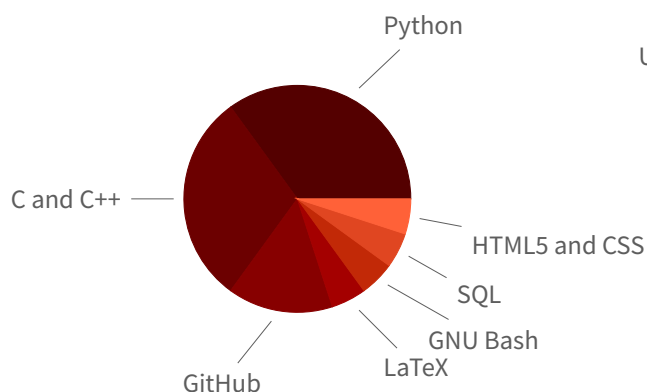
UCSF Chimera, Maestro, AmberTools, GOLD, MDTraj, OpenMM, VMD, Desmond, Glide
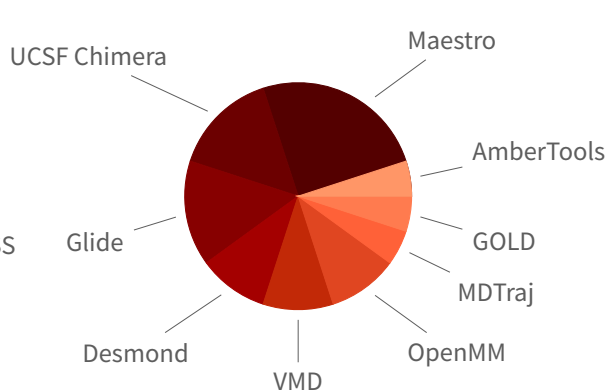
Positions

Ph.D. position in PELE development   *Barcelona, Spain*

Barcelona Supercomputing Center, Life Sciences department   *Sep. 2018 - PRESENT*

- Design of a new algorithm to sample the effects of interfacial water molecules in protein-ligand simulations.
- Research and development of new strategies and algorithms to estimate binding free energies through Monte Carlo simulations and the free energy perturbation technique.
- Application of computational methods in enzyme engineering studies.

Software developer intern at the Electronic and Atomic Protein Modeling Group   *Barcelona, Spain*

Barcelona Supercomputing Center, Life Sciences department   *Feb. 2018 - Aug. 2018*

- Design of a new algorithm to sample the effects of interfacial water molecules in protein-ligand simulations.

Student collaborator at Insilichem   *Barcelona, Spain*

Universitat Autònoma de Barcelona, Chemistry department   *Feb. 2016 - Feb. 2017*

- Research on improving docking predictions for metal containing systems.

International mobility

Visit to the William L. Jorgensen Research Group   *New Haven, United States of America*

Yale University, Department of Chemistry   *Dec. 2018*

Research visitor at the University of Notre Dame

Notre Dame, United States of America

CHEMISTRY AND BIOCHEMISTRY DEPARTMENT

Sep. 2016 - Dec. 2016

- Modelling and Development of a transition state force field and its applications to an artificial suzukiase.
- This research visit was planned with the support of the Programa Propi de Pràctiques mobility program of the Universitat Autònoma de Barcelona.

Publications

PELE-MSM: A Monte Carlo Based Protocol for the Estimation of Absolute Binding Free Energies

2019

J. Chem. Theory Comput. 15, 6243–6253   *10.1021/acs.jctc.9b00753*   ⦿ *NostrumBioDiscovery/msm_pele*

Joan F. Gilabert, Christoph Grebner, Daniel Soler, Daniel Lecina, <u>Martí Municoy</u>, Oriol Gracia Carmona, Robert Soliva, Martin J. Packer, Samantha J. Hughes, Christian Tyrchan, Anders Hogner, Victor Guallar

Selective synthesis of 4-hydroxyisophorone and 4-ketoisophorone by fungal peroxygenases

2019

Catal. Sci. Technol. 9, 1398–1405   *10.1039/c8cy02114g*

Carmen Aranda, <u>Martí Municoy</u>, Víctor Guallar, Jan Kiebist, Katrin Scheibner, René Ullrich, José C. del Río, Martin Hofrichter, Angel T. Martínez, Ana Gutiérrez

GaudiMM: A modular multi-objective platform for molecular modeling

2017

J. Comput. Chem. 38 (24), 2118-2126   *10.1002/jcc.24847*   ⦿ *insilichem/gaudi*

Jaime Rodríguez-Guerra, Giuseppe Sciortino, Jordi Guasp, <u>Martí Municoy</u>, Jean-Didier Maréchal

Conference talks

5th BSC Severo Ochoa Doctoral Symposium

Barcelona, Spain

PRESENTER FOR SAMPLING INTERFACIAL WATER EFFECTS OVER PROTEIN SPECIFICITY WITH PELE

Apr. 2018

Honors & Awards

2019	**FI Ph.D. grant**, Generalitat de Catalunya	*Barcelona, Spain*
2016	**Programa propi pràctiques**, Universitat Autònoma de Barcelona	*Barcelona, Spain*
2009	**Joves i Ciència program**, Fundació Catalunya La Pedreda, 2nd promotion	*Barcelona, Spain*