# Martí **Municoy Terol**

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## Education

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

Universitat Autònoma de Barcelona — *2017 - 2018*

- Specialization in Data Science

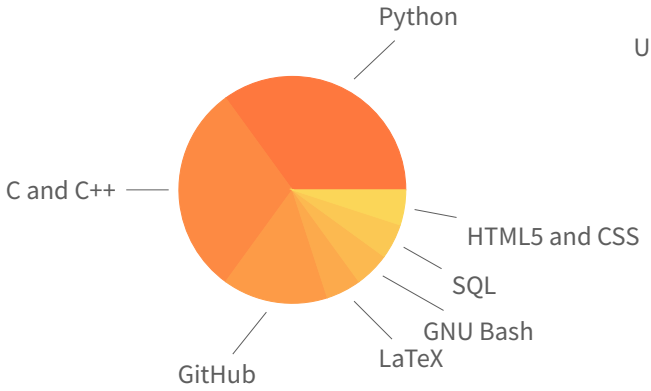
**B.Sc. in Chemistry** — *Barcelona, Spain*

Universitat Autònoma de Barcelona — *2011 - 2017*

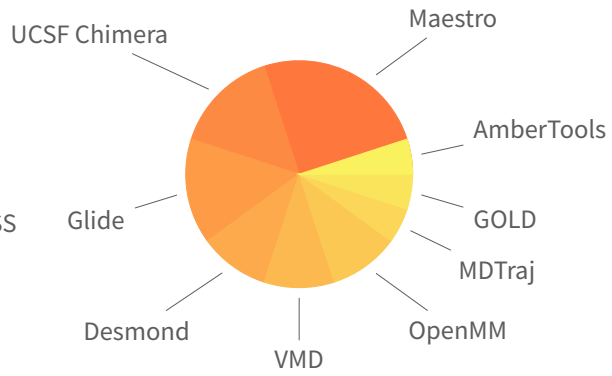
**B.Sc. in Physics** — *Barcelona, Spain*

Universitat Autònoma de Barcelona — *2011 - 2017*

## Programming skills

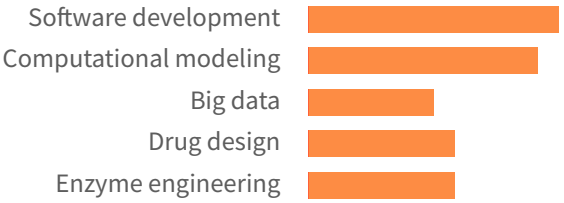



## Scientific software




## Languages


## Interests




## 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, U.S.A*

Yale University, Department of Chemistry *Dec. 2018*

**Research visitor at the University of Notre Dame** *Notre Dame, U.S.A*

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, Martí Municoy, 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, Martí Municoy, 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, Martí Municoy, 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*