

# Martí Municoy Terol

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## Education

### M.Sc. in Modelling for Science and Engineering

UNIVERSITAT AUTÒNOMA DE BARCELONA

- Specialization in Data Science

Barcelona, Spain

2017 - 2018

### B.Sc. in Chemistry

UNIVERSITAT AUTÒNOMA DE BARCELONA

Barcelona, Spain

2011 - 2017

### B.Sc. in Physics

UNIVERSITAT AUTÒNOMA DE BARCELONA

Barcelona, Spain

2011 - 2017

## Positions

### Ph.D. position in PELE development

BARCELONA SUPERCOMPUTING CENTER, LIFE SCIENCES DEPARTMENT

- 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.

Barcelona, Spain

Sep. 2018 - PRESENT

### Software developer intern at the Electronic and Atomic Protein Modeling Group

BARCELONA SUPERCOMPUTING CENTER, LIFE SCIENCES DEPARTMENT

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

Barcelona, Spain

Feb. 2018 - Aug. 2018

### Student collaborator at Insilichem

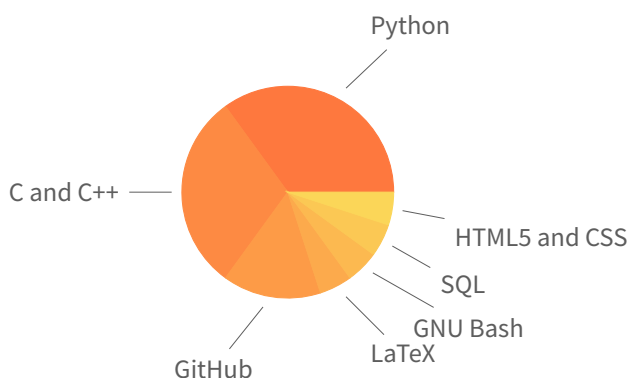
UNIVERSITAT AUTÒNOMA DE BARCELONA, CHEMISTRY DEPARTMENT

- Research on improving docking predictions for metal containing systems.

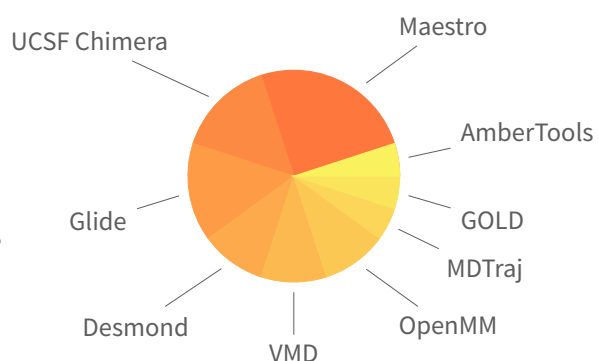
Barcelona, Spain

Feb. 2016 - Feb. 2017

## Programming skills



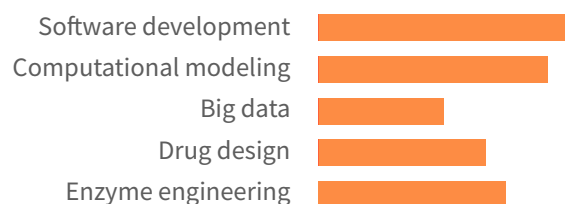
## Scientific software



## Languages



## Interests



## International mobility

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### Visit to the William L. Jorgensen Research Group

YALE UNIVERSITY, DEPARTMENT OF CHEMISTRY

New Haven, U.S.A

Dec. 2018

### Research visitor at the University of Notre Dame

CHEMISTRY AND BIOCHEMISTRY DEPARTMENT

Notre Dame, U.S.A

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

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### 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 Muncioy, 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 Muncioy, Víctor Guallar, Jan Kiebitz, 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 Muncioy, Jean-Didier Maréchal

## Conferences

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### Alchemical Free Energy Workshop 2019

Göttingen, Germany

POSTER PRESENTER FOR ESTIMATION OF ABSOLUTE AND RELATIVE BINDING FREE ENERGIES WITH PELE

May. 2019

### 5th BSC Severo Ochoa Doctoral Symposium

Barcelona, Spain

TALK PRESENTER FOR SAMPLING INTERFACIAL WATER EFFECTS OVER PROTEIN SPECIFICITY WITH PELE

Apr. 2018

## Honors & Awards

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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 Pedrera, 2nd promotion

Barcelona, Spain