

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

Director Business Solutions

NOSTRUM BIODISCOVERY

- Coordinating the development of technology solutions at NBD.
- Combining them all under the NBD Suite®, the place where NBD's molecular modelling and machine learning software is unified, automatized and standardized.

Barcelona, Spain

Feb. 2021 - PRESENT

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

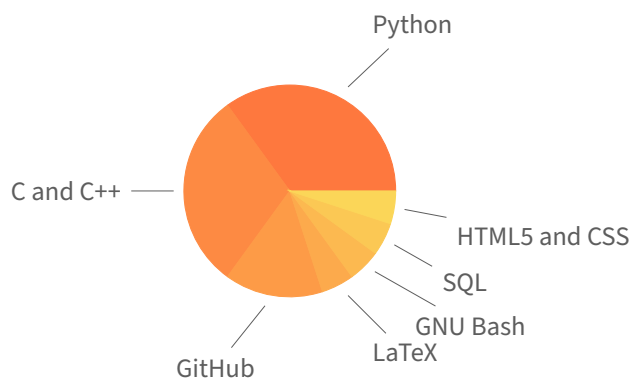
UNIVERSITAT AUTÒNOMA DE BARCELONA, CHEMISTRY DEPARTMENT

- Research on improving docking predictions for metal containing systems.

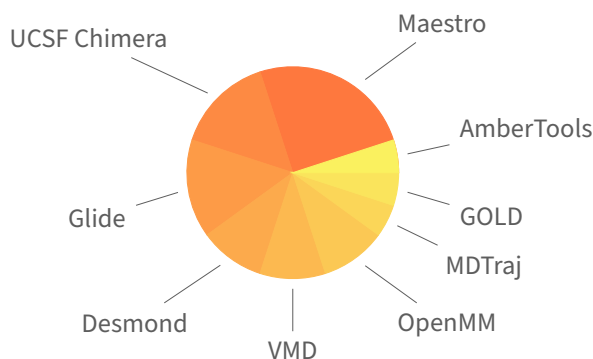
Barcelona, Spain

Feb. 2016 - Feb. 2017

Programming skills



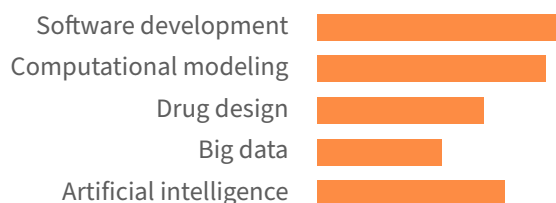
Scientific software



Languages



Interests



International mobility

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

aquaPELE: A Monte Carlo-Based Algorithm to Sample the Effects of Buried Water Molecules in Proteins

2020

J. Chem. Theory Comput. 2020, 16, 12, 7655–7670 10.1021/acs.jctc.0c00925

Martí Muncioy, Sergi Roda, Daniel Soler, Alberto Soutullo, Victor Guallar

Fatty-Acid Oxygenation by Fungal Peroxygenases: From Computational Simulations to Preparative Regio- and Stereoselective Epoxidation

2020

ACS Catal. 2020, 10, 22, 13584–13595 10.1021/acscatal.0c03165

Martí Muncioy, Alejandro González-Benjumea, Juan Carro, Carmen Aranda, Dolores Linde, Chantal Renau-Mínguez, René Ullrich, Martin Hofrichter, Victor Guallar, Ana Gutiérrez, Angel T. Martínez

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 peroxxygenases

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

Alchemical Free Energy Workshop 2019

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

Göttingen, Germany

May, 2019

5th BSC Severo Ochoa Doctoral Symposium

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

Barcelona, Spain

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