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*

Positions

Director of Technology Office   *Barcelona, Spain*

NOSTRUM BIODISCOVERY   *Feb. 2021 - PRESENT*

- Coordinating the development of technology solutions at Nostrum Biodiscovery
- Development of the Nostrum Suite®, the place where Nostrum's molecular modelling and artificial intelligence software is unified, automatized and standardized
- Management of the corporate High Performance Computing infrastructure combining on-premise and cloud-based on-demand resources

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.
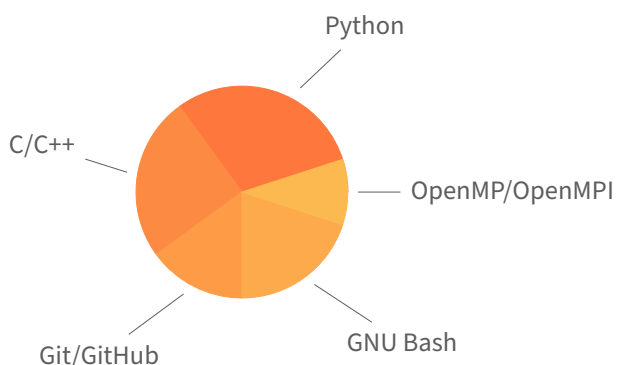
Student collaborator at Insilichem   *Barcelona, Spain*

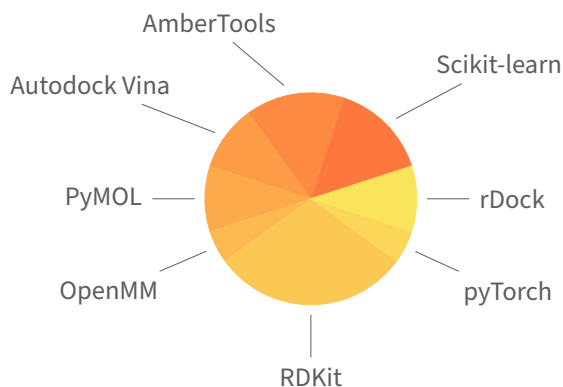UNIVERSITAT AUTÒNOMA DE BARCELONA, CHEMISTRY DEPARTMENT   *Feb. 2016 - Feb. 2017*

- Research on improving docking predictions for metal containing systems.

Programming skills

Scientific software

Languages

English
Spanish
Catalan

Interests

Software development
Computational modeling
Artificial intelligence
High performance computing
Cloud computing

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

High-Throughput Prediction of the Impact of Genetic Variability on Drug Sensitivity and Resistance Patterns for Clinically Relevant Epidermal Growth Factor Receptor Mutations from Atomistic Simulations

2023

J. Chem. Inf. Model. 2023, 63, 1, 321–334   *10.1021/acs.jcim.2c01344*

Aristarc Suriñach, Adam Hospital, Yvonne Westermaier, Luis Jordà, Sergi Orozco-Ruiz, Daniel Beltrán, Francesco Colizzi, Pau Andrio, Robert Soliva, <u>Martí Municoy</u>, Josep Lluís Gelpí, Modesto Orozco

Selective inhibitors of the PSEN1–gamma-secretase complex

2023

J. Biol. Chem. (2023) 299(6) 104794   *10.1016/j.jbc.2023.104794*

Lutgarde Serneels, Rajeshwar Narlawar, Laura Perez-Benito, <u>Martí Municoy</u>, Victor Guallar, Dries T'Syen, Maarten Dewilde, François Bischoff, Erwin Fraiponts, Gary Tresadern, Peter W. M. Roevens, Harrie J. M. Gijsen, Bart De Strooper

Combining machine-learning and molecular-modeling methods for drug-target affinity predictions

2022

WIREs Comput Mol Sci. 2022;e1653   *10.1002/wcms.1653*

Carles Perez-Lopez, Alexis Molina, Estrella Lozoya, Victor Segarra, <u>Martí Municoy</u>, Victor Guallar

Pre-exascale HPC approaches for molecular dynamics simulations. Covid-19 research: A use case

2022

WIREs Comput Mol Sci. 2022;e1622   *10.1002/wcms.1622*

Miłosz Wieczór, Vito Genna, Juan Aranda, Rosa M. Badia, Josep Lluís Gelpí, Vytautas Gapsys, Bert L. de Groot, Erik Lindahl, <u>Martí Municoy</u>, Adam Hospital, Modesto Orozco

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*

<u>Martí Municoy</u>, 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*

<u>Martí Municoy</u>, 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, <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

Conferences

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

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*