

# Pablo Herrera Nieto

Researcher

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📍 Madrid

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## Profile summary

Five years of experience on basic research as data analyst focused on biological data. My professional goal is to apply precise and state-of-the-art data science approaches to real-world health problems.

## Skills

### Programming

python  
javascript  
R  
bash  
L<sup>A</sup>T<sub>E</sub>X  
html, css  
sql, mongodb

### Software

numpy, pandas, matplotlib,  
scikit-learn  
tidyverse

### Data analysis

clustering  
dimensionality reduction  
markov models

### Operating systems

linux  
windows

### Languages

spanish (native)  
english (advanced)

## Experience

### Universidad Autónoma de Madrid (Spain)

**Postdoctoral Researcher** | Supervisor: Ramón Díaz Uriarte  
February 2021-Present

- Implemented simulations algorithms for cancer evolution.
- Supervised Master students.

### Universitat Pompeu Fabra (Barcelona, Spain)

**Data Analyst | PhD** | Supervisor: Gianni de Fabritiis  
June 2016-July 2020

- Authored 3 publications.
- Handled high-throughput computing resources.
- Built predictive models from time-series data sets using clustering, dimensionality reduction methods, and Markov state models.
- Assisted in the development of a novel reinforcement learning algorithm for conformational sampling of proteins.
- Studied complex biological processes related to intrinsically disordered proteins.

### Janssen | Johnson & Johnson (Toledo, Spain)

**Junior Computational Chemistry Researcher**  
September 2015-May 2016

- Analyzed the structural role of water in GPCRs.
- Developed homology models.
- Completed virtual screening campaigns.

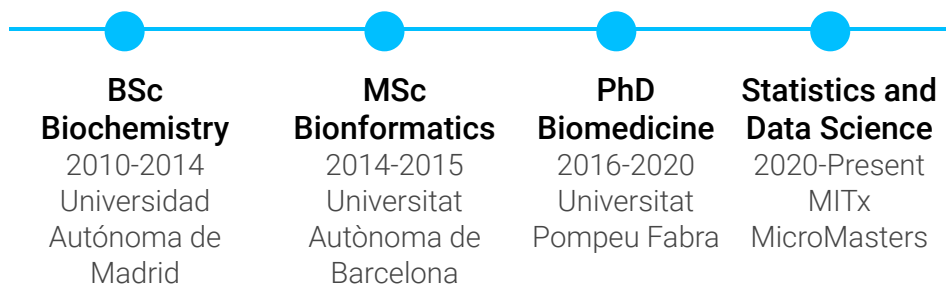
### Universitat Autònoma de Barcelona (Spain)

**Master student**

February 2015-September 2015

- Constructed homology models of GPCRs.

## Education



## Impact

### Selected Publications

- Adrià Pérez, Pablo Herrera-Nieto, Stefan Doerr, and Gianni De Fabritiis. "AdaptiveBandit: A Multi-armed Bandit Framework for Adaptive Sampling in Molecular Simulations" Journal of Chemical Theory and Computation 16.7 (2020): 4685-4693.
- Pablo Herrera-Nieto, Adrià Pérez, and Gianni De Fabritiis. "Characterization of partially ordered states in the intrinsically disordered N-terminal domain of p53 using millisecond molecular dynamics simulations" Scientific reports (2020)