Pablo Herrera Nieto

Researcher

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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
LaTeX
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

BSc Biochemistry
2010-2014
Universidad Autónoma de Madrid

MSc Bionformatics
2014-2015
Universitat Autònoma de Barcelona

PhD Biomedicine
2016-2020
Universitat Pompeu Fabra

Statistics and Data Science
2020-Present
MITx MicroMasters

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)