

Ismael Rodríguez

Bioinformatics &
Ancient proteins

Contact

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- 📱 LinkedIn

Skills

Python & R

- Jupyter, Quarto, Shiny, Plotly
- R for MS, pyOpenMS, Pyteomics

Systems

- Linux & Git
- High Performance Computing

Palaeoproteomics data analysis

- LC-MS/MS
- MALDI-TOF ZooMS
- Open search, *de novo*

Statistics & ML

- Statistical modelling
- Deep learning and LLMs

Education

09/2021 - 12/2024

PhD in Palaeoproteomics
University of Cambridge

09/2017 - 09/2019

MSc in Bioinformatics
University of Copenhagen

09/2012 - 07/2016

BSc in Biotechnology
Technical University of Madrid

Languages

- **Spanish**
Native
- **English**
Fluent, scientific and professional
- **Portuguese**
Fluent conversation

Experience

PlaCe ITN MSCA-ERC PhD - Ancient proteins

09/2021 - 12/2024

Department of Archaeology -
McDonald Institute for Archaeological Research
University of Cambridge

I developed software packages and pipelines to process mass spectrometry data on ceramics, bone and parchment. I pioneered the use of *open search* software for LC-MS/MS and R and Python for high throughput analysis of ZooMS data.

Research Assistant - Ancient proteins

04/2020 - 09/2021

Globe Institute
University of Copenhagen

Within the Beasts2Craft project, I carried out computational analysis of ZooMS MALDI-TOF and LC-MS/MS data for palaeoproteomics. My tasks also involved server administration.

Research Assistant - scRNA-seq Transcriptomics

06/2019 - 12/2019

Department of Biomedical Sciences
University of Copenhagen

Using R, I analyzed single-cell RNA-seq to understand molecular mechanisms, especially those impacting ion channels, involved in heart remodelling in arrhythmia.

Master thesis student in Palaeoproteomics

04/2019 - 10/2019

Globe Institute
University of Copenhagen

Thesis: Assessing deamidation patterns in collagen from ancient sites by mining mass-spectrometry data.
Bioinformatics Project: Methodological comparison of Hi-C and shotgun sequencing data from ancient samples

Student Assistant - RNA-seq Transcriptomics

05/2018 - 05/2019

Department of Biomedical Sciences
University of Copenhagen

I conducted novel analysis of miRNA-mRNA networks involved in structural remodelling of the heart in arrhythmia. I analysed and integrated RNAseq and miRNA microarray transcriptomics data using R and Python.

Teaching

Supervisor - BA (Hons) Archaeology

10/2022 - 5/2023

University of Cambridge

Conducting small group sessions with undergraduates to work on exercises, essays and explore topics further.

Practicals coordinator - Palaeoproteomics Summer School

8/2021

University of Copenhagen

Organising, teaching and conducting practical palaeoproteomics sessions.

HPC and Linux workshops

3/2021

University of Copenhagen

Organising and delivering workshops on Linux and HPC and R.

Dissemination

Care and Conservation of Manuscripts 20th seminar

Arnamagnæan Institute, Department of Nordic Studies and Linguistics

ZooMS data reveals variation in parchment manufacturing methods over a millenium

Arch-Sci Pitt-Rivers Seminars

Department of Archaeology. University of Cambridge

Challenges, approaches and insights on palaeoproteomic analysis on ceramics

Integrating ZooMS and Zooarchaeology, methodological challenges and interpretive potentials

University of Kent

High-throughput analysis and batch effect in ZooMS MALDI-TOF data

PAASTA monthly talks

Palaeoproteomics and Archaeology, Society for Techniques and Advances

Benchmarking the identification of a single degraded protein to explore optimal search strategies for ancient proteins

EuBIC-MS Winter School 2022

European Bioinformatics Community for Mass Spectrometry

Parchment Glutamine Index (PQI): A novel method to estimate glutamine deamidation levels in parchment collagen obtained from low-quality MALDI-TOF data

Projects

This is a list of software projects for ZooMS and LC-MS/MS in palaeoproteomics. See my github profile for a comprehensive list of open source projects.

R and Python data analysis for ZooMS

DataAnalysisZooMS (Quarto Web), RegExTractor, MALDIzooMS and MALDIpqi (packages)

Suite of R and Python workflows to process and analyze MALDI-TOF data for ZooMS on parchment and bone

Python packages for proteomics.

MSMSdeamidation, PalaeoPSM, setMQrun, PPbenchmark

Tools to set up software runs for and process LC-MS/MS, PSM and PTM data.

The Archaeoriddle challenge.

Archaeoriddle book, Archaeoriddle package

Assessing quantitative methods in archaeology via simulated datasets.

Publications

- [1] Viñas-Caron Laura C; Rodriguez Ismael et al. "A biological reading of a palimpsest". In: *iScience* (Apr. 29, 2023), p. 106786. ISSN: 2589-0042. DOI: 10.1016/j.isci.2023.106786.
- [2] Nair Bharath; Rodriguez Ismael et al. "Parchment Glutamine Index (PQI): A novel method to estimate glutamine deamidation levels in parchment collagen obtained from low-quality MALDI-TOF data". In: *Peer Community J.* 3 (e10 Jan. 18, 2023). ISSN: 2804-3871. DOI: 10.24072/pcjournal.230.
- [3] Bethencourt Jorsua Herrera; Rodriguez Ismael et al. "Data from A biocodicological analysis of the medieval library and archive from Orval abbey, Belgium". In: *J. Open Archaeol. Data* 10 (0 Feb. 22, 2022). ISSN: 2049-1565,2049-1565. DOI: 10.5334/joad.89.
- [4] Rodriguez Ismael; Nair Bharath et al. "Benchmarking the identification of a single degraded protein to explore optimal search strategies for ancient proteins". In: *bioRxiv, recommended by Peer Community In* (Sept. 19, 2024), p. 2023.12.15.571577. DOI: 10.1101/2023.12.15.571577.
- [5] Rodriguez Ismael; Ogawa Thimotee et al. "The role of the ceramic fabric in the preservation and recovery of proteins". In: *In preparation* (2025).
- [6] Rodriguez Ismael; Nair Bharath. "Data analysis for ZooMS". In: *In preparation* (2025).
- [7] A Cortell-Nicolau et al. "Assessing quantitative methods in archaeology via simulated datasets: The Archaeoriddle challenge. Concept, project and motivations". en. In: *J. Archaeol. Sci.* 177 (106179 May 2025), p. 106179. ISSN: 0305-4403,1095-9238. DOI: 10.1016/j.jas.2025.106179.
- [8] Ntasi Georgia; Rodriguez Ismael et al. "Molecular signatures written in bone proteins of 79 AD victims from Herculaneum and Pompeii". In: *Sci. Rep.* 12 (1 May 27, 2022), p. 8401. ISSN: 2045-2322,2045-2322. DOI: 10.1038/s41598-022-12042-6.
- [9] Larupa Santos Joana; Rodriguez Ismael et al. "Transcriptome analysis of a pig model of sustained atrial fibrillation using bulk and single-nucleus RNA-sequencing". In: *Under review* ().
- [10] Larupa Santos Joana; Rodríguez Ismael et al. "Investigating gene-microRNA networks in atrial fibrillation patients with mitral valve regurgitation". In: *PLoS One* 15 (5 May 11, 2020), e0232719. ISSN: 1932-6203. DOI: 10.1371/journal.pone.0232719.