



# Peer Community In Mathematical & Computational Biology

## Systematic investigation of software tools and design of a tailored pipeline for paleoproteomics research

**Raquel Assis** based on peer reviews by **Shevan Wilkin**  and 1 anonymous reviewer

Ismael Rodriguez-Palomo, Bharath Nair, Yun Chiang, Joannes Dekker, Benjamin Dartigues, Meaghan Mackie, Miranda Evans, Ruairidh Macleod, Jesper V. Olsen, Matthew J. Collins (2024) Benchmarking the identification of a single degraded protein to explore optimal search strategies for ancient proteins. bioRxiv, ver. 3, peer-reviewed and recommended by Peer Community in Mathematical and Computational Biology.

<https://doi.org/10.1101/2023.12.15.571577>

Submitted: 12 March 2024, Recommended: 21 October 2024

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Paleoproteomics is a rapidly growing field with numerous challenges, many of which are due to the highly fragmented, modified, and degraded nature of ancient proteins. Though there are established standards for analysis, it is unclear how different software tools affect the identification and quantification of peptides, proteins, and post-translational modifications. To address this knowledge gap, Rodriguez Palomo et al. design a controlled system by experimentally degrading and purifying bovine beta-lactoglobulin, and then systematically compare the performance of many commonly used tools in its analysis.

They present comprehensive investigations of false discovery rates, open and narrow searches, de novo sequencing coverage bias and accuracy, and peptide chemical properties and bias. In each investigation, they explore wide ranges of appropriate tools and parameters, providing guidelines and recommendations for best practices. Based on their findings, Rodriguez Palomo et al. develop a proposed pipeline that is tailored for the analysis of ancient proteins. This pipeline is an important contribution to paleoproteomics and is likely to be of great value to the research community, as it is designed to enhance power, accuracy, and consistency in studies of ancient proteins.

### References:

Ismael Rodriguez-Palomo, Bharath Nair, Yun Chiang, Joannes Dekker, Benjamin Dartigues, Meaghan Mackie, Miranda Evans, Ruairidh Macleod, Jesper V. Olsen, Matthew J. Collins (2023) Benchmarking the identification of a single degraded protein to explore optimal search strategies for ancient proteins. bioRxiv, ver.3 peer-reviewed and recommended by PCI Math Comp Biol  
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## Reviews

### Evaluation round #2

#### Reviewed by anonymous reviewer 1, 07 October 2024

I thank Palomo et al. for their thoughtful responses to my reviews. The physicochemical section is excellent. I'm happy that you included the isoelectric point and other properties. I think it really strengthens the observed results and will be helpful for similar future preservational studies on other proteins.

#### Reviewed by [Shevan Wilkin](#) , 17 October 2024

The authors have adjusted all of the comments I requested. The paper reads well and is extremely thorough. I would recommend the manuscript at this point.

The only "issue" I have is that the proposed pipeline includes several searches using multiple platforms for each sample, which exponentially increases the time and work to complete any study. Hopefully some researchers incorporate this pipeline into new work so we can see the how much these additional steps add to the reliability of ancient protein studies.

### Evaluation round #1

DOI or URL of the preprint: <https://doi.org/10.1101/2023.12.15.571577>

Version of the preprint: 2

#### Authors' reply, 20 September 2024

[Download author's reply](#)

#### Decision by [Raquel Assis](#), posted 23 July 2024, validated 24 July 2024

##### Major revision

The submitted manuscript is an important contribution to paleoproteomics. However, the reviewers have identified several issues with the clarity of the manuscript text and figures. I recommend that the authors carefully address these on a point-by-point basis, particularly as this manuscript should serve as a guide for best practices in paleoproteomics.

#### Reviewed by anonymous reviewer 1, 03 May 2024

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Reviewed by **Shevan Wilkin** , 22 July 2024

Please see my attached document with comments. Please feel free to contact me with any questions. Apologies if anything isn't clear - I just returned from holiday am down with COIVD...

Shevan

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