



UNIVERSITY OF LEEDS

This is a repository copy of *Mechanisms of Peptide Oxidation by Hydroxyl Radicals: Insight at the Molecular Scale*.

White Rose Research Online URL for this paper:
<http://eprints.whiterose.ac.uk/116519/>

Version: Supplemental Material

Article:

Verlackt, CCW, Van Boxem, W, Dewaele, D et al. (5 more authors) (2017) Mechanisms of Peptide Oxidation by Hydroxyl Radicals: Insight at the Molecular Scale. *The Journal of Physical Chemistry C*, 121 (10). pp. 5787-5799. ISSN 1932-7447

<https://doi.org/10.1021/acs.jpcc.6b12278>

© 2017 American Chemical Society. This document is the Accepted Manuscript version of a Published Work that appeared in final form in *The Journal of Physical Chemistry C*, copyright © American Chemical Society after peer review and technical editing by the publisher. To access the final edited and published work see <https://doi.org/10.1021/acs.jpcc.6b12278>.

Reuse

Unless indicated otherwise, fulltext items are protected by copyright with all rights reserved. The copyright exception in section 29 of the Copyright, Designs and Patents Act 1988 allows the making of a single copy solely for the purpose of non-commercial research or private study within the limits of fair dealing. The publisher or other rights-holder may allow further reproduction and re-use of this version - refer to the White Rose Research Online record for this item. Where records identify the publisher as the copyright holder, users can verify any specific terms of use on the publisher's website.

Takedown

If you consider content in White Rose Research Online to be in breach of UK law, please notify us by emailing eprints@whiterose.ac.uk including the URL of the record and the reason for the withdrawal request.



eprints@whiterose.ac.uk
<https://eprints.whiterose.ac.uk/>

Supplementary Information

Mechanisms of peptide oxidation by hydroxyl radicals: insight at the molecular scale

C. C. W. Verlackt^[a], W. Van Boxem^[a], D. Dewaele^[b], F. Lemièrè^[b], F. Sobott^[b,c,d], J. Benedikt^[e], E C Neyts^[a], A Bogaerts^{*[a]}

- a. Research group PLASMANT, Department of Chemistry, University of Antwerp, Universiteitsplein 1, 2610 Antwerp, Belgium
- b. Biomolecular & Analytical Mass Spectrometry group, Department of Chemistry, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerp, Belgium
- c. Astbury Centre for Structural Molecular Biology, University of Leeds, Leeds, UK
- d. School of Molecular and Cellular Biology, University of Leeds, Leeds, UK
- e. Research Department Plasmas with Complex Interactions, Ruhr-Universität Bochum, 44780 Bochum, Germany

* Corresponding authors: annemie.bogaerts@uantwerpen.be

T: +32-(0)3-265.23.77

Figure S-1. Summary of the Covariance Values After 1 μ s for Native Peptide A and Peptide A Containing an Increasing Amount of Oxidized Amino Acids (A-Tyr, A-ox2 and A-ox3, Respectively). Non-Reactive Simulations of the Third Step of the Investigation Were Performed a Second Time for the Given Structures to Investigate the Expected Fluctuations on the Calculated Values.

Peptide A	
Structure	Covariance value (nm^2)
A-Nat	15.87
A-Tyr	7.59
A-ox2	20.68
A-ox3	17.04

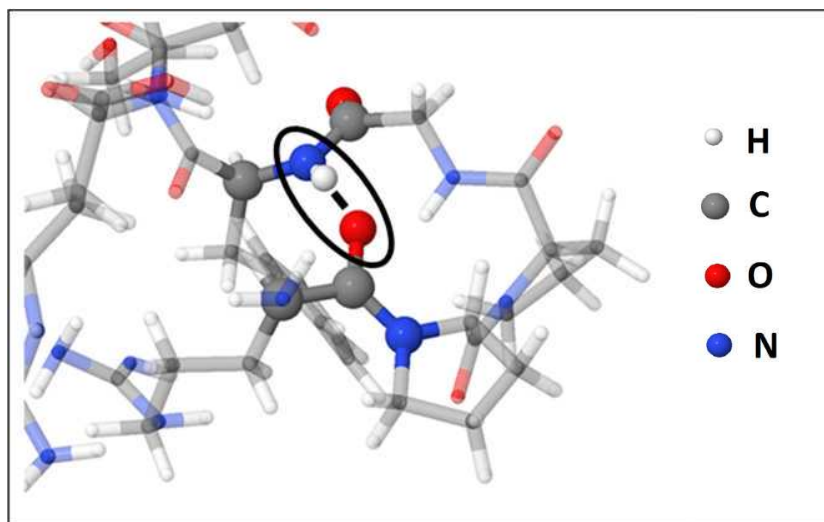


Figure S-2. Example of a site where the intrapeptide interaction is observed in peptide B (indicated by a black line in the circle). The interacting site is depicted using solid spheres while the remaining peptide of the snapshot is shown using a semitransparent stick model.

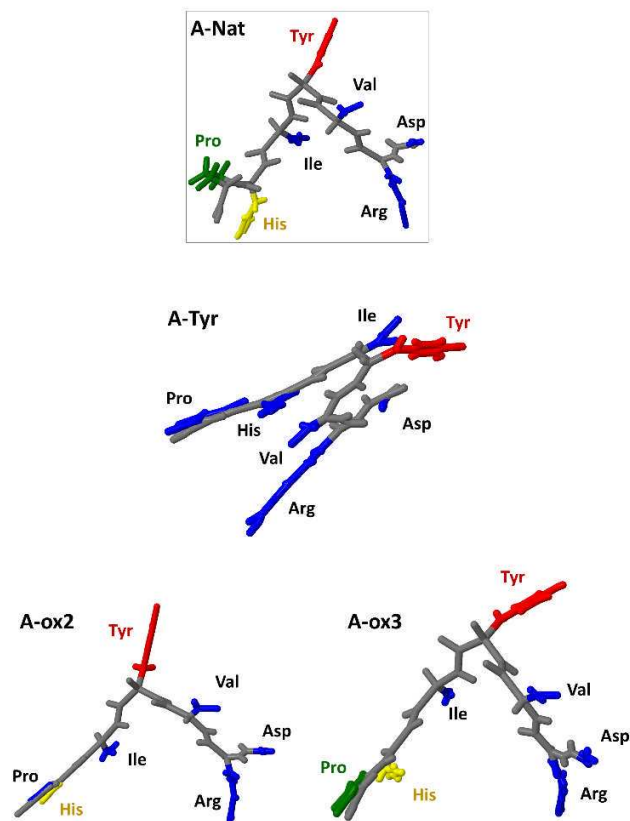


Figure S-3. Representation of the average structures of the native peptide A (grey box) and peptide A containing an increasing amount of oxidized amino acids (A-Tyr, A-ox2 and A-ox3, respectively). The peptide backbone is depicted in grey using a stick model in all structures. Un-oxidized amino acid side groups are depicted in blue. Red, yellow and green indicate the oxidation of Tyr, His and Pro, respectively. These average structures are obtained from the second batch of long-term MD calculations in order to verify the repeatability of the simulations.