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Supplementary Information

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

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Figure S-1. Summary of the Covariance Values After 1 μs 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

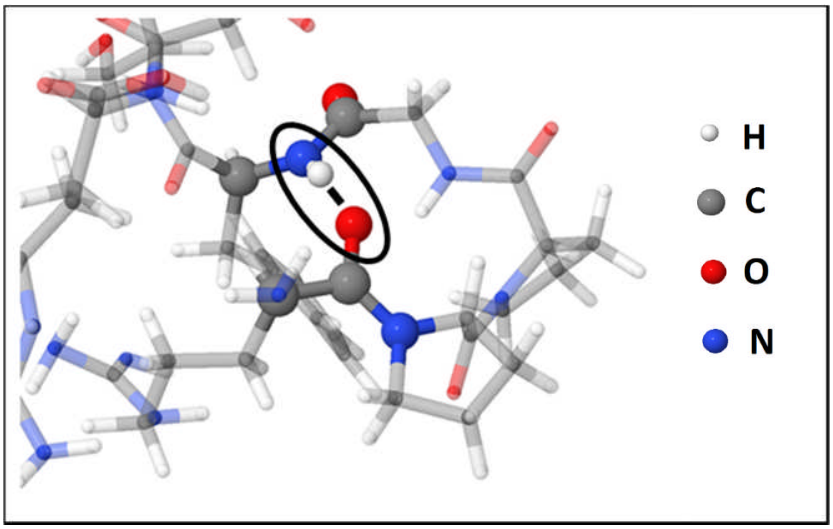

Figure S-2. Example of a site where the intrapeptide interaction is observed in peptide B (indicated by a black line in the circle). The interacting site is depicted using solid spheres while the remaining peptide of the snapshot is shown using a semitransparent stick model.

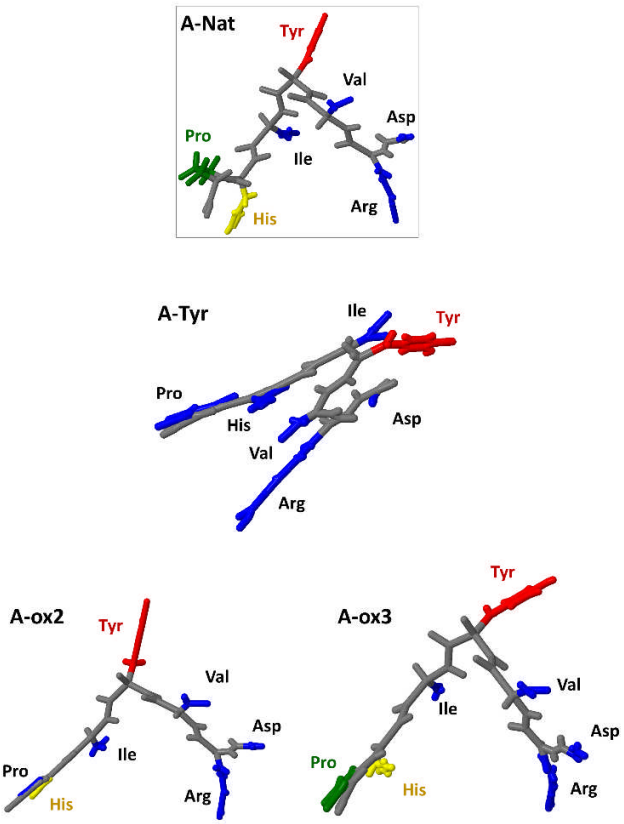

Figure S-3. Representation of the average structures of the native peptide A (grey box) and peptide A containing an increasing amount of oxidized amino acids (A-Tyr, A-ox2 and A-ox3, respectively). The peptide backbone is depicted in grey using a stick model in all structures. Un-oxidized amino acid 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.