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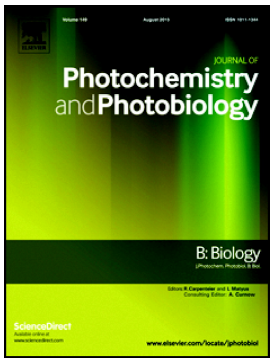

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Methionine oxidation by hydrogen peroxide in peptides and proteins: a theoretical and Raman spectroscopy study

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Abstract

The oxidation of proteins results in their deterioration via the oxidation of reactive amino acids. Oxidation of the amino acid, methionine plays an important role during biological conditions of oxidative stress, and equally a role in protein stability. In this study the oxidation of the methionine residue using the tripeptide GlyMetGly with respect to hydrogen peroxide has been studied using both Raman spectroscopy and DFT calculations. Spectral modifications following the formation of methionine sulfoxide are shown with the appearance of the S=O vibration whilst there is also the modification of the C-S vibrations at approximately 700 cm^{-1}. The changes in the intensity of the C-S stretching band were used to calculate the kinetic rate constant as $7.9 \pm 0.6 \times 10^{-3}$ dm^3 mol^{-1} s^{-1}. The energy barrier for the reaction. is determined both experimentally and using DFT calculations. The reaction of the dairy protein beta-lactoglobulin with hydrogen peroxide is equally studied using the same technique. The solvent accessible surface area of the methionine residues within the protein were also