

demonstrates a synergistic effect between the two compounds, apparently resulting from inhibition of AP-1 signaling. Taken together, these results suggest that the co-administration of Cy3glc and 5-ASA could be a potential strategy to control inflammation in IBD.

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Unexpected reactions of the reducing alpha-aminoalkyl radical in the oxidation of S-alkyl-glutathiones

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Laser flash photolysis and high-resolution mass spectrometry were used to investigate stable modifications of S-alkyl-glutathione peptides from the one-electron oxidation by triplet 3-carboxybenzophenone. The tripeptides studied were S-methyl-glutathione and S-ethyl-glutathione, and they have shown very similar behavior. Two major intermediates involved in stable product formation were identified as an α -thioalkyl radical and an α -aminoalkyl radical. The α -aminoalkyl radical formation proceeds via formation of a 9-membered (SN)-type cyclic radical with the participation of an amino group on the gamma-Glu residue as the precursor for decarboxylation. This reducing α -aminoalkyl radical undergoes an electron-transfer reaction in the presence of 3-carboxybenzophenone yielding a resonance-stabilized carbocation which, in turn, undergoes an intramolecular ring-closure forming a stable product as identified by high-resolution mass spectrometry (LC-MS/MS) technique. These biologically-relevant reaction paths yielding stable peptide modifications are reported in this work for the first time.

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Development of antimicrobial protein-based polymers for biomedical applications

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Inspired in naturally occurring fibrous proteins and composed of amino acid building blocks commonly found in structural proteins, protein-based polymers (PBPs) are a group of materials with unique chemical, physical and biological properties. Conventional recombinant DNA

technology allows the biological synthesis of recombinant protein-based polymers (rPBPs) with precise control over its size and composition and the incorporation of functional bioactive domains such as antimicrobial peptides (AMPs). Owing to the unique balance between their mechanical properties, biocompatibility, biodegradability and thermostability, elastin-like recombinamers (ELRs) and silk-elastin like proteins (SELPs) are two of the most remarkable families of rPBP for biotechnological applications. Here, we describe the functionalization of a SELP and an ELR with different antimicrobial peptides that showed promising results against several Gram-positive and Gram-negative bacterial strains. This will provide the basis for the development of advanced biomaterials processed into different types of structures (e.g. hydrogels, films, fibers, particles) suitable for biomedical applications.

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Molecular determinants of the influenza fusion peptide activity

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The emergence of an influenza pandemic is one of the biggest health threats of our time and there is an urgent need to develop vaccines and drugs against a broad spectrum of influenza viruses (IV). A promising strategy to combat IV is to inactivate the fusion process between the viral and host membranes, which is mediated by the surface protein hemagglutinin (HA). During this process, the N-terminal region of HA, known as fusion peptide (FP), inserts into the host membrane. Although it has been shown that the FP plays a crucial role in the fusion process, the molecular effect of the peptide remains unclear. To analyse the molecular determinants underlying the IV FP, we used state of the art simulation techniques, including metadynamics and constant pH molecular dynamics. The simulation results were combined spectroscopic methods to analyse the peptide's affinity for lipid membranes and its ability to promote lipid-mixing. This allowed us to obtain a detailed molecular characterization of the peptide's conformational properties and its effect on the host membrane. Our work also sheds light into the effect of mutations and external conditions, such as pH, on the FP activity. These results can be useful for the design of novel therapies against this devastating pathogen.

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