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## Quantitative mass spectrometry for nutritional peptidomics: Evaluating the impact of food processing technology by multivariate statistical approaches

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Assessing the nutritional quality of dietary proteins is important for formulating public health policies. Food processing technologies can modify protein structure and therefore can impact their gastrointestinal digestion, leading to different bioaccessibility outcomes. Heat-induced protein aggregation is a modification that commonly occurs during food processing and physicochemical conditions during heating determine the final aggregate structure. The present study aimed to investigate the impact of aggregate structure, using 5 different heating conditions, on the nature and amount of peptides released from an egg protein during *in vitro* digestion.

Mass spectrometry experiments were performed on the protein digests using a Q-exactive mass spectrometer. More than 15000 peptide identifications were generated, corresponding to 593 unique peptide sequences, which were quantified.

Quantitative data analysis was performed by LDA, a supervised multivariate analysis. The clustering analysis performed on the discriminant scores resulted in 6 homogenous clusters of peptides; each cluster was defined by a specific concentration profile depending on the initial protein/aggregate structure. Therefore, the nature of peptides released is driven by aggregation conditions, which modulate enzyme accessibility. Some masking/unmasking mechanisms of specific protein zones are hypothesized. The conclusions resulting from these analyses, combined with a precise characterization of the quantified peptides, made it possible to predict the conformational modifications occurring during protein aggregation.

Consequently, based on advanced statistical analysis of quantitative mass spectrometry data, it was possible to demonstrate that physicochemical modifications during protein heating impact the further digestion process. Since the resulting peptide profile can be modified, significant nutritional consequences are expected.