Monitoring iron speciation during gastrointestinal digestion: X-ray Absorption Spectroscopy

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Iron is a micronutrient involved in critical metabolic processes, such as the oxygen and electron transportation, the cellular division and their differentiation and the energy metabolism, among others. However, the shift towards plant-based diets, coupled with sustainability issues in the food system, food insecurity, and the scarcity of affordable, sustainable sources of nutrition, has resulted in a lack of attention being given to micronutrient deficiencies. The World Health Organization (WHO) estimates that iron deficiency affects over 1.2 billion people worldwide and remains a global challenge to treat. Therefore, understanding the effect of digestion on iron at a molecular level is vital for developing effective, sustainable nutritional interventions.

This study investigated the impact of digestion on iron speciation in food. In this study, heme iron from myoglobin was selected as the 'gold standard' food source as it has been shown to be more easily absorbed than non-heme iron. All samples underwent an in vitro gastrointestinal digestion process in accordance with the standardised INFOGEST protocol. The effect of digestion on iron speciation was then monitored using advanced X-ray absorption spectroscopy (XAS).

Preliminary results confirm that heme iron maintains its state (XANES) during digestion. Additionally, EXAFS analysis revealed that there were dynamic structural adaptations during digestion: while non-digested myoglobin exhibited octahedral coordination, gastric conditions caused distorted 5-coordinate geometry, with complete reversion to octahedral coordination after the intestinal stage. These reversible changes suggest a protective mechanism that preserves iron absorption while allowing the necessary structural flexibility during the gastrointestinal digestive process.
This is the first time that the behavior of heme iron has been characterized at a molecular level during complete *in vitro* digestion, providing detailed insights into its structural transformations. This study demonstrates the indispensable utility of XAS in nutritional iron research and contributes to the multiscale understanding of nutrient behavior in food systems

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XAS, iron, digestion, speciation

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