



Evaluation of Protein Profiles, Bioactivity, Allergenicity and Toxicity of Peptides Generated After in silico Digestion of Common Wheat and Einkorn Wheat

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ABSTRACT

The belief that ancient wheat is more beneficial than common wheat has been growing trend in recent years among the consumers. The present study aims to compare bioactive peptide, allergen peptide and toxic peptide generation after gastrointestinal digestion of modern wheat (*Triticum aestivum*) and ancient wheat, einkorn (*Triticum monococcum* var. *monococcum*), using in silico tools. The primary sequences of both kinds of wheat were obtained from BIOPEP-UWM and UniProtKB/Swiss-Prot database. In silico digestion was applied using BIOPEP-UWM online tool. For the simulation of gastrointestinal digestion pepsin (pH 1.3) (EC 3.4.23.1), trypsin (EC 3.4.21.4), and chymotrypsin (EC 3.4.21.1) were selected and analyzed. Homology analysis was performed for each protein sequences using EMBOSS Needle program. Toxic and allergen peptides were predicted using ToxinPred online tool and Allergen FP v.1.0. The results showed that einkorn and common wheat proteins exhibited similar properties including high similarity rate (58.72-87.40%) indicating the percentage of matches between the two sequences and the identical bioactivities for peptides generated after digestion. Most of the bioactive peptides were dipeptides and the majority of them displayed more than one bioactivities including ACE inhibitory, DPP IV inhibitory or antioxidant activity, etc. Allergen peptides generated after in silico digestion were found to be similar for both kinds of wheat. In silico gastric digestion of einkorn and wheat caused toxic peptides production, but they were disappeared after in silico intestinal digestion. In conclusion, although there is a perception related to the Einkorn that is healthier than common wheat, in silico digestion of common wheat and einkorn did not support this perception.

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