

Title (8)	:	Exploring the Potential of Black Soldier Fly Larval Proteins as Bioactive Peptide Sources through in Silico Gastrointestinal Proteolysis: A Cheminformatic Investigation
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Abstract	:	Despite their potential as a protein source for human consumption, the health benefits of black soldier fly larvae (BSFL) proteins following human gastrointestinal (GI) digestion are poorly understood. This computational study explored the potential of BSFL proteins to release health-promoting peptides after human GI digestion. Twenty-six proteins were virtually proteolyzed with GI proteases. The resultant peptides were screened for high GI absorption and non-toxicity. Shortlisted peptides were searched against the BIOPEP-UWM and Scopus databases to identify their bioactivities. The potential of the peptides as inhibitors of myeloperoxidase (MPO), NADPH oxidase (NOX), and xanthine oxidase (XO), as well as a disruptor of Keap1–Nrf2 protein–protein interaction, were predicted using molecular docking and dynamics simulation. Our results revealed that about 95% of the 5218 fragments generated from the proteolysis of BSFL proteins came from muscle proteins. Dipeptides comprised the largest group (about 25%) of fragments arising from each muscular protein. Screening of 1994 di- and tripeptides using SwissADME and STopTox tools revealed 65 unique sequences with high GI absorption and non-toxicity. A search of the databases identified 16 antioxidant peptides, 14 anti-angiotensin-converting enzyme peptides, and 17 anti-dipeptidyl peptidase IV peptides among these sequences.