Streamlining Bioactive Peptide Discovery With In Silico Prospecting: An investigation on Seaweed Pacific Dulse

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Objectives: Bioactive hydrolysates and peptides from seaweed sources have been shown to exert beneficial effects in both in vitro and in vivo models for metabolic health. However, the discovery approach relies heavily on the conventional hydrolysate preparation and screening model selection, both driven by resource availability and time constraints. Considering the potential for functional food and therapeutics development, efficient and cost-effective strategies are needed to scope out as much prospect that can be screened for increased chances of hits to find potent, stable, and commercializable bioactive peptides (BAPs). This work aimed to identify multifunctional BAPs from seaweed Pacific Dulse, and to determine which hydrolytic condition can favor the release of more BAPs of interest from this protein-rich macroalgae.

Methods: Virtual hydrolysates were prepared from dulse proteins using three digestion platforms (ExPASy, SystemsBio, and Rapid Peptide Generator) under three production stream contexts (hydrolysate preparation, gastrointestinal digestion, and microbial fermentation). Peptide products were then subjected to *in silico* bioactivity prospecting for anti-inflammatory, antidiabetic, and antihypertensive potential. Stability in the intestine and blood was predicted along with potential toxicity. Non-toxic and stable peptides predicted to have multifunctionalities were shortlisted for bioactivity validation, and production streams predicted to generate most number of BAPs were noted for test hydrolysate production.

Results: With our approach, we identified 13 novel prospect BAPs that have multiple bioactivities, high stability, and low toxicity. Hydrolysate production using bromelain and ficin favored the 5–10aa long mBAPs generation. Simulated gastrointestinal digestion and microbial fermentation also showed promise in the release of some BAPs of interest.

Conclusions: When consumed in either hydrolyzed, whole, or fermented form, BAPs can be generated from seaweed Pacific Dulse proteins. Bioactivity testing of the novel BAPs identified, and microscale production of the promising BAP production stream are underway.

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