Carnosine-related dipeptides as potential therapeutics against cancer: in silico estimation of activity, synthesis and in vitro analysis

Klaudia Chmielewska[1], Justyna Budka[2], Szymon Kowalski[2], Mateusz Daśko[1], Katarzyna Kozlowska-Tylingo[1], Krystyna Dzierzbicka[1], and Iwona Inkielewicz-Stepniak[2]

[1]Gdańsk University of Technology
[2]Medical University of Gdansk

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Abstract

Background and purpose: Peptides constitute an interesting starting point for drugs, although research on them is quite slowed by the fact that most of them are non-patentable. Given that carnosine, β-Ala-His dipeptide, was found useful in cancer treatment, we aimed to inspect whether its similar structures could also possess such activity. Experimental Approach: The interdisciplinary approach allows for the much more detailed analysis, hence our study presents computational analysis of potential targets and therapeutic activities of dipeptides with β-Ala or His at the N-end, synthesis and in vitro cytotoxicity and apoptosis tests against a chosen cancerous and non-cancerous cell line. Key Results: We preliminarily propose β-Ala-Ala, His-Val and His-Arg as most potent entities, in regard to carnosine, a known anticancer peptide. Conclusion and Implications: An interdisciplinary approach allows for a much more complex analysis and in silico tests should be a standard element of every toxicological report and we hope to popularize that concept worldwide. Peptides indeed possess activity against cancer, with little to no harm to non-cancerous cells, which is highly valuable.

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