International Journal of
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Computational Approaches to Bioactive Peptide Prediction and Discovery

Guest Editor:

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Deadline for manuscript submissions:
closed (31 May 2023)

Message from the Guest Editor

Peptides derived from the hydrolysis of naturally occurring proteins are known to contain a large number of interesting bioactivities (antidiabetic, antihypertensive, antimicrobial, etc.). Therefore, a first goal of the current Special Issue is to describe the state of the art of the computational tools that can be used for this bioactivity prediction. This includes, but is not limited to, protein–peptide docking tools, protein–peptide complex free-energy prediction, and deep/machine-learning approaches. In all cases, only manuscripts that contain a computational or in vitro assessment of the reliability of their predictions will be considered for peer review.

The second goal of this Special Issue is to emphasize web servers and databases that help to discover easy ways: (1) to obtain a specific bioactive peptide from available sources; (2) to obtain different bioactive peptides from a specific protein source.

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Message from the Editor-in-Chief

The International Journal of Molecular Sciences (*IJMS*, ISSN 1422-0067) is an open access journal, which was established in 2000. The journal aims to provide a forum for scholarly research on a range of topics, including biochemistry, molecular and cell biology, molecular biophysics, molecular medicine, and all aspects of molecular research in chemistry. *IJMS* publishes both original research and review articles, and regularly publishes special issues to highlight advances at the cutting edge of research. We invite you to read recent articles published in *IJMS* and consider publishing your next paper with us.

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