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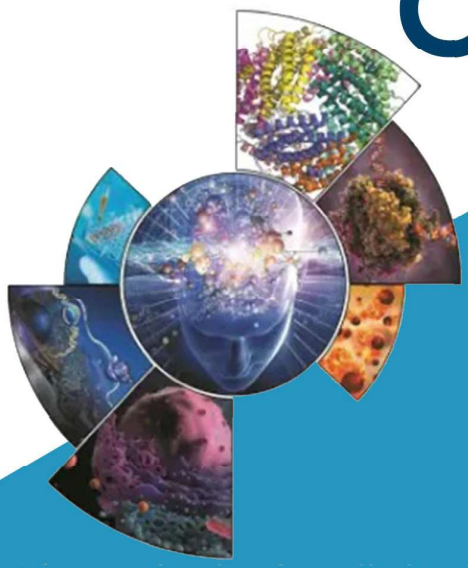
ANNUAL BIOINFORMATICS CONFERENCE 2022



DISCUSSIONS AND INSIGHTS

MAJOR TOPICS

- System Biology
- Big Data in Biology
- Structural Bioinformatics
- Biological Sequences Analysis
- AI & Machine Learning in Biology
- Modeling in Computeational Biology
- Computational Drug Design & Discovery

1st International and 10th National Iranian Conference on Bioinformatics

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Molecular docking of Enterocin-P peptide with DNA: an in silico study

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Abstract

Antibiotic resistance is a looming public health crisis especially in animal industry. Hence, researchers are looking for natural alternatives such as Antimicrobial peptides (AMPs). Nowadays, AMPs, also known as host defense peptides, are short and generally positively charged peptides found in a wide variety of life forms from microorganisms to humans. One of the modes of action of some AMPs were the binding with DNA and can directly affect the expression of related genes and inhibit the synthesis of macromolecules or destroy. Among AMPs Entrocin-P peptide has attracted a lot of attention from researchers. The aim of this study was to evaluated the possibility of binding DNA to Entrocin-P peptide. The structure of Entrocin-p peptide was obtained from previous study. A general strategy for docking and modelling DNA–protein complexes has been developed with HADDOCK server. HADDOCK uses non-structural experimental data to drive the docking during a rigid-body energy minimization, and semi-flexible and water refinement stages. The latter allow for flexibility of all DNA nucleotides and the residues of the protein at the predicted interface. Using this method, we have reproduced the structure of Entrocin-P peptide bound to DNA. The results have shown that the model of the Entrocin-P -DNA complex successfully has predicted. Furthermore, the results indicated that interactions were occurred by the major groove of DNA with α-helix part of this peptide. The best haddock score was -74.3 +/- 3.5. In addition, the value of Z-Score was -2.5. Its Z-score indicates how many standard deviations from the average this cluster is located in terms of score that the more negative the better.

Key Words: *Entrocin-P, Peptide, Bioinformatics, DNA, Molecular docking*