# عنوان مقاله:

Evaluation the mechanism of binding of CLF۳۶ chimeric peptide to DnaK and OmpC into the surface proteins in Gram-negative bacteria using computer-based methods

### محل انتشار:

چهارمین کنگره بین المللی و شانزدهمین کنگره ملی ژنتیک (سال: 1399)

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#### خلاصه مقاله:

Background and Aim: Antibiotic resistance results same problems related to human health. One of the new ways for replacing antibiotic is using antimicrobial peptides. CLF\(\mathbb{P}\)F is a lactoferrin drived chimeric peptides from camel milk, which has a higher potential antimicrobial activity than Lactoferin. Although antimicrobial peptides have multiple function, but their potential for intracellular targets is still not clear. The purpose of present study was to investigate the antimicrobial effect of CLF\(\mathbb{P}\)F peptides on some important surface protein in Gram negative bacteria such as DnaK and OmpC. Methods: At the first step appropriate structure for surface protein was obtained from CLF\(\mathbb{P}\)F protein and peptide database. after that, for molecular docking, preparation of surface proteins and peptide chimer CLF\(\mathbb{P}\)F was performed by using UCSF chimera software. Clus pro Y.\(\sigma\) bioinformatics softwarewas used for stimulation of intracellular interaction of CLF\(\mathbb{P}\)F peptides and PDF file was evaluated by pymol software. Results: Bioinformatics analysis results indicated that molecular interaction of CLF\(\mathbb{P}\)F peptide with DnaK and OmpC surface proteins which studied peptide, which has amino acids that have a lowest binding energy, formed a strong hydrogen binding bacterial surface proteins. Conclusion: Based on obtained results it can predicted that CLF\(\mathbb{P}\)F chimeric peptide is capable to counteracting Gram-negative bacteria and as a result, they are effective in reducing reduce their pathogenicity and it will be a good alternative for substitution by antibiotics, but for confirmation and providing accurate results it require

# كلمات كليدى:

Antimicrobial peptides, Chimeric peptide CLFWF, Surface proteins, Molecular interaction

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