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OF MEDICAL SCIENCES



# ANNUAL BIOINFORMATICS CONFERENCE 2022



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## The investigation of horse myostatin with human follistatin by molecular docking method

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### Abstract

Myostatin is a transforming growth factor-beta (TGF-beta) family member that plays roles as a negative regulator of muscle mass development. Follistatin is a myostatin-binding protein that can inhibit myostatin activity to promote muscle growth. This is an important way for increasing growth especially in demo horses. Here, we aimed to prediction inhibition activity of equine myostatin protein with human follistatin, through bioinformatics tools. The Swiss-model server was applied to predict the third (three-dimensional) structure of horse myostatin protein and studies with SAVES 6.0 online server. After that, the interactions of myostatin with human follistatin were evaluated using variety of tools such as Verify3D, ERRAT and ClusPro2.0 online software [2, 3]. The results showed that the Verify3D for this protein was at least 88% of the amino acid residues have an average score of  $3D-1D > = 0.2$ , which is acceptable for our protein. strategy evaluates proteins using a three-dimensional structure. This score varies from -1 (poor score) to +1 (good score). ERRAT is an online server that confirms the structure of a protein on the assumption of nuclear fusion between different types of atoms, with total quality index in this study was 83.52 which is acceptable. According to the Ramachandarn plot, for horse myostatin 88.7% of the amino acids in this structure were in the desired region, which is acceptable for predicting the third structure. The docking result showed that the N-terminal of follistatin was in contact with TGF-beta region in myostation that related to myostatin activity according to crystallography structure, derived from the docking of human follistatin with mouse myostatin. Finally, our research indicated that the binding energy in our predicted model was -903 which is close to the result of binding energy of the docking human follistatin with mouse myostatin which is reported -1323.3.

**Key Words:** *Follistatin, Equus caballus, Myostatin, Bioinformatics, Molecular Docking*

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