Abstract

Introduction

Boswellic acid is one of the five ring triterpene compounds that is obtained from the gemresin of *Boswellia serrata* and *Boswellia carteri*. Boswellic acid is one of the compounds that has an effect on the treatment and prevention of Alzheimer's and strengthens memory. In this study, new targets that boswellic acid and its derivatives can be affected were evaluated.

Material and methods

In the present project, 800 different proteins that are affected by boswellic acid and its derivatives were received from the PDB site. Then different steps and filters were applied on Proteins. Finally, their energy and interactions were investigated using Autodock software.

Results

Derivatives Acetyl-α-Boswellic Acid and Acetyl-lupeolic Acid were bounded to the active site of estrogen receptor protein with high binding free energy of -10.40 and -11.13 kcal/mol, and 9,11-dehydro-α-Boswellic Acid، Acetyl-9,11-dehydro-α-Boswellic Acid، Lupeolic acid، Acetyl-11-keto-β-Boswellic Acid، 11-keto-β- Boswellic Acid respectively with free binding energy of -9.10, -9.72, -9.72, -10.67 and -10.38 kcal/mol with high affinity for the active site of PI3K enzyme.

Discussion and conclusion

In a recent study to identify and introduce new protein targets of boswellic acid, the estrogen receptor protein and the enzyme PI3K, which had the best binding to boswellic acid and its derivatives, were identified and introduced. Evaluation of the interactions of these proteins with boswellic acid and its derivatives showed that the amino acids Met804, Ile963, Asp964, Asp950, Met953, Ser806 and Asn951 may play an important role in binding these compounds to the active site of PI3K enzyme. It also seems that the amino acids Met343, Met421, Phe404, Met388, Leu387, Leu391, Arg394, Leu384, Glu353, Leu346, Leu349, Leu525 and His524 may play an important role in binding these compounds to the active site of the estrogen receptor protein.

Keywords: Boswellic acid, Inverse Docking, Z-Score