STUDY ON THE EFFECT OF TWO NEW PHENOLIC COMPOUNDS ON THE ACTIVITY OF HUMAN SALIVARY ALPHA-AMYLASE

N.alipour saqa[1], sh. Khalil- Moghaddam [2]*, A.shahvelayati[3]
[1,2]Department of Biology, Yadegar-e-Imam Khomeini (RAH) Shahre Rey Branch, Islamic Azad University, Tehran, Iran
[3]Department of chemistry, Yadegar-e-Imam Khomeini (RAH) Shahre Rey Branch, Islamic Azad University, Tehran, Iran
*shiva.moghaddam@yahoo.com

Abstract: Carbohydrate digestion has been targeted as a mean to control postprandial increase of blood glucose [1]. Inhibitors of carbohydrate digesting enzymes, such as alpha-amylase and alpha-glucosidase, are now actively searched for, since they could ultimately make useful medicines against diabetes and obesity[2,3].

Although powerful synthetic inhibitors of starch digestive enzymes, such as acarbose, are available to control postprandial hyperglycemia, new synthetic inhibitors are investigated too.The objective of this study was to evaluate the α-amylase inhibitory activity of two new phenol- ninhydrin derivatives (monoadduct ninhydrin pyrogallol and bis adduct ninhydrin pyrogallol) using in silico docking studies. Acarbose, a known α-amylase inhibitor was used as the standard. In silico docking studies were carried out using recent version of AutoDock 4.2, which has the basic principle of Lamarckian genetic algorithm. Additional molecules to 1SMD.pdb, including solvent, were deleted prior to docking. The docking box was positioned at x = 6.805, y = 49.167, z = 12.297 with a size of 70x70x70. A docking experiment suggests the existence of a common binding site for the two derivatives (in active site). Interactions between enzyms and inhibitors was pi-pi and hydrogen bonds. In order to get an approximation of the possible effectiveness of these ligands as a potential inhibitor of the enzyme, docking score was obtained for the 1SMD.pdb and two new phenol- ninhydrin derivatives. This score was −9 kcal/mol for monoadduct and −8.20 kcal/mol for bis adduct. In comparison, acarbose had a score of −11.04 kcal/mol, which is suggesting that our ligands could inhibit amylase activity.

Keywords: diabetes; Human salivary alpha amylase; ninhydrin pyrogallol derivatives

References

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