**INVESTIGATION OF THE EFFECTS OF 16-DEOXYSAIKOGENIN F AND JUGLONE COMPOUNDS ON PANCREATIC CHOLESTEROL ESTERASE ENZYME IN SILICO AND IN VITRO**

**Sevki Adem**

**Department of Chemistry, Faculty of Science, Cankiri Karatekin University, 18100 Cankırı, Türkiye**

**Zeyad Adıl Hameed Hameed**

**Department of Chemistry, Faculty of Science, Cankiri Karatekin University, 18100 Cankırı,Türkiye**

|  |
| --- |
| **ABSTRACT**  High blood cholesterol levels are a major problem for blood vessels. High levels cause cardiovascular problems, which are among the leading causes of death in our country. Pancreatic cholesterol esterase plays an important role in the hydrolysis and absorption of dietary cholesterol from the small intestine. This enzyme is considered a therapeutic target to reduce the amount of dietary cholesterol. In this study, we investigated the effects of some natural compounds on the enzyme in vitro. Enzyme activity was measured spectrophotometrically. The inhibition effect on the enzyme was determined in five different concentrations of 16-Deoxysaikogenin F and Juglone compounds. IC50 values were calculated from the % activity-concentration graphs. At the same time, docking studies were performed to understand through which interactions the inhibitory compounds might have prevented the enzyme activity.  Pancreatic esterase enzyme activity was inhibited by 16-Deoxysaikogenin F and Juglone compounds with IC50 values of 61.340 and 86.64, respectively. In the docking study, the affinities of the molecules towards the active site of the enzyme were determined as -102.168 and -56.5749 MOlDock Score, respectively. |

# Keywords: *Pancreatic cholesterol esterase, 16-Deoxysaikogenin F and, Juglone*