



UNIVERSITY OF ZABOL

Faculty of Science

Department of Chemistry

Subject:

Investigating the molecular docking of a number of flavonoid compounds with cyclin-dependent kinase on colon cancer cells

Supervisors

Dr. Mansour Ghaffari Moghaddam

Dr. Esmael Sanchooli

Advisors

Dr. Hojjat Samrah Delarami

Dr. Mansoureh Rakhshanipour

By:

Elahe Amjadian

Winter

1401

Abstract

Colon cancer refers to the growth of cancerous cells in the colon. This disease occurs due to abnormal and uncontrolled cell growth. Cyclin-dependent kinase is a protein kinase that plays a role in regulating the cell cycle. Abnormal activity of cyclin-dependent kinase is associated with cancer progression and metastasis. Epidemiological studies have shown that regular consumption of flavonoids is beneficial in preventing the transformation of normal cells into cancer cells. The aim of this study was to use flavonoid compounds to inhibit cyclin-dependent kinase in the treatment of colon cancer. In this research, the structure of certain flavonoid derivatives was optimized using quantum calculations. Then, molecular docking of these derivatives with cyclin-dependent kinase enzymes with codes 6GUE and 2A4L was performed using the MOE software, and the results of molecular docking were analyzed. As expected, *van der Waals* interactions and hydrogen bonds of these derivatives with the enzyme, particularly with the 6GUE code, played an important role in inhibiting this enzyme.

Keywords: Molecular docking, Flavonoid, Cyclin-dependent kinase, Colon cancer