Investigating the Avermectin Family Compounds Against Tubulin Protein: A Molecular Docking Study

P-28-017

Q. Hoti *[I], U.M. Ghali *[II], S. Adem[II], K. Hoti[I], F. Gavazaj[I]

[I]College of Medical Science ‘’REZONANCA’’, Pristina, Kosovo, [II]Faculty of Science, Department of Chemistry, Çankiri Karatekin University, Çankiri, Türkiye

The Avermectins belong to the 16-membered macrocyclic lactone family, which includes ivermectin, abamectin, moxidectin, milbemycin oxime, doramectin, selamectin, and eprinomectin. The recent findings regarding the anticancer activity of avermectins have provided additional impetus to studies on their application for treatment. These compounds are predicted to have anticancer effects on several cell lines. The objective of this study is to utilize in silico approaches to investigate the avermectin family compound's therapeutic potential against the tubulin protein. Molecular docking analyses were performed using tubulin protein (PDB: 1TUB) on the CB-Dock 2 webserver and visualized using PyMol software. The attached ligands were removed using Notepad++, and SWISSMODE was employed to build a template for missing amino acid residues. Interestingly, the results revealed that all the avermectin family compounds displayed higher binding scores compared to the reference anticancer drug, taxol. The compound ivermectin B1a, followed by doramectin, eprinomectin, and selamectin, exhibited the highest scores of -8.8, -8.7, -8.7, and -8.7 Kcal/mol, respectively. The present work provides scientific evidence that these avermectin compounds could be considered potential candidates for the development of anticancer drugs targeting tubulin protein in the future.

* The authors marked with an asterisk equally contributed to the work.