

Abstract

# Synthesized a New Organic Compound's Cytotoxic Activity Quantum Mechanics Calculations and Docking Studies <sup>†</sup>

Senem Akkoç, Burçin Türkmenoğlu \* and Sevtap Çağlar Yavuz

Department of Chemistry, Faculty of Sciences, Erciyes University, Kayseri 38039, Turkey; senemakkoc@erciyes.edu.tr (S.A.); scaglar@erciyes.edu.tr (S.C.Y.)

\* Correspondence: bkilic@erciyes.edu.tr; Tel.: +90-506-831-0727

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**Abstract:** There are many drugs currently on the market which are organic compounds and natural products. Various coordination compounds have been extensively studied in the chemotherapy treatment of cancer. For finding an effective anticancer drug, a new organic compound synthesized and characterized. The cytotoxic effect of the synthesized compound against MDA-MB-231 and DLD-1 cell lines using *in vitro* 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide assays measured in terms of their IC<sub>50</sub> values. According to obtained results, new compound have anticancer activity toward both breast and colon cancer cell lines with low IC<sub>50</sub> values and it will be more developed for *in vivo* studies in the near future. The theoretical calculations of this active molecule also were performed in this study. This molecule has examined using the Spartan 10 package program with the DFT method (B3LYP). By determining the most appropriate conformer of the molecule, data about stable structure was obtained. Furthermore, molecular docking studies were performed to elucidate the attachment patterns and properties of ligand. For the molecular docking study, the Glide module method of the Schrodinger Suite was utilized. From the best docking exposures, it was determined which amino acid residues of this ligand interacted with active residues.

**Keywords:** organic compound colon cancer; breast cancer; cytotoxic activity; docking study



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