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In-Silico comparative studies of the effect of Metformin and Geraniol on GPC1 protein in Endometrial Cancer

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***Abstract*—** endometrial cancer (EC) is the fourth most known carcinoma worldwide in females. Geraniol (GER) is one of the acyclic monoterpene alcohols that got from essential oils of aromatic plants. Metformin is the first-line medication that is recommended for patients with type 2 diabetes. Newly, metformin has acquired an interest as an anti-cancer agent in a few carcinoma types, despite the fact that studies in EC are limited. Glypican 1 (GPC1) is highly expressed in malignant tumors. The 3D structure of the targeted protein GPC1 (PDB ID: 4YWT) was obtained from the PDB online database. In-silico Molecular docking compounds analysis is performed in PyRx software with the AutoDock Vina software. All compounds used in this study demonstrated significant anticancer activity against EC by binding to the inhibitor site of GPC1 protein. The result displayed the good potency as an inhibitor to GPC1with the optimum binding energy of -4, 5 kcal/mol in drug metformin and significantly -4, 9 kcal/ mol in Geraniol compounds. These results predict that metformin and Geraniol might have the potential as an anti-carcinoma against EC and could be developed to treat cancer.

Key words: Endometrial cancer, Glypican 1, Metformin, Molecular Docking

I. Introduction

Endometrial cancer (EC) is the most common leading cancer in females from developed countries with about 100,000 new cases in 2012[1]. This tumor growth begins in the internal layer of the uterus when epithelial cells covering the myometrium begin to abnormally multiply. Even though, most ECs are diagnosed in the early stages, predominantly because of suggestive postmenopausal metrorrhagia, up to 20 percent of the lesions progress to high-stage cancer. Unfortunately, in this situation, the five-year survival in these cases drops to 15 percent, compared to 90 percent in groups of females diagnosed with confined disease. The presence of disseminated aggressive endometrial cancer cells and myometrial infiltration are necessary events for prognosis and death in patients[2]. The prognosis of stage I disease is overall considered to be as good an outcome of surgical treatment. Furthermore, the prognosis of the advanced stage of the disease (IV or III) is poor, with a 5-year general survival rate fluctuating between 47-69% and somewhere in the range of 15-17% in various studies[3]. Thusly, it is crucial to prevent the occurrence of gynecological cancers[4]. This study predicting the prognosis of EC has used Cancer Genome Atlas (TCGA). Glypican 1(GPC1) protein expression increases in EC. Recently GPC1 has received developing interest cause of its high capability of visualizing tissues that are soft [5-7]. GPC1is a heparan sulfate proteoglycan (HSPG) whose expression in normal tissues is mostly restricted to the ovary and testis[8]. It has been reported that GPC1is one of the genes associated with glycolysis and related to overall survival. The importance of identifying new therapies for cancers especially EC is warranted due to its stability and association with insulin resistance, obesity, and diabetes, which increase a female's risk of developing[9-11].