Evaluation of Sesquiterpenes from Ferula assa-foetida on inflamatory parameters and study of biding modes using computational methods

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Abstract

introduction: Ferula assafoetida is a source of sesquiterpenes [1]. According to an investigation, phenolic compounds at physiological concentration can inhibit inflammatory enzymes [2]. These enzymes digest the extracellular matrix and provide the conditions for activation and migration and proliferation of endothelial cells. Reported studies on medicinal plants for their inhibitory effect on MMP are very limited.

Methods and Results:

Acetone extract of plant was prepared and Sesquiterpenes were purified using HPLC preparative analyses and their structures were elucidated. After culturing the cell at confluence, cells were isolated and the supernatant was removed. The pure substances were applied on cell lines U87MG and Wehi activities. Besides the structure has been docked in the active site of metalloproteinase, and significant interactions were determined.Subsequently, ligand-protein complexes were subjected to molecular dynamics simulation in water and thermodynamic properties were calculated. In the phytochemistry field galbanic acid, mogoltadone, kellerin, polyanthin and polyanthininwere produced from F. assafoetida. The results of celluar toxicity study shows that IC50 of Galbanic acid, Mogoltadone and Polyanthin in Wehi cell line were 925.2703, 721.86, and 680.3 µg/ml in U87MG cell line were 952.193, 752.352, 678.742. Galbanic acid, mogoltadone, kellerin, polyanthin and polyanthininwere solated from F. assafoetida. The results of celluar toxicity study show that IC50 of Galbanic acid, Mogoltadone and Polyanthin in Wehi cell line were 925.2703, 721.86, and 680.3 µg/ml in U87MG cell line were 952.193, 752.352, 678.742

Conclusion: Investigation revealed that the coumarins have inhibitory effects on the content and activity of MMP 2.9 and showed anti-angiogenetic effect. So, they can be potentially effective in the treatment of cancer. Interactive and competitive binding between MMP-9 and Galbanic acid were studied with FT-IR, UV-Vis and fluorescence methods and MMP-9 structure was changed in these interactions.

Keywords: Galbanic acid, Mogoltadone, Kellerin, Polyanthin, Matrix metalloproteinases