University of Zabol
Graduate School

Faculty of Agriulture
Department of Plant Breeding and Biotechnology
The Thesis Submitted for the Degree of Ph.D.

Virtual screening in TCM database to find key molecules inhibitors of colorectal inflammation pathway with molecular dynamics: an approach to cell culture and next generation sequencing

Supervisor:

Dr. B.A. Fakheri
Dr. A.A. Bahari

Advisors:

Dr. N. Mahdinezhad

By:
Ali Sargazi

winter 2022

Abstract

Traditional Chinese medicine is an essential part of the medical science of several Asian countries and plays a role as a complementary medicine in many western countries. Its purpose is to create a holistic approach to maintaining health and trying to provide harmony of body and mind. Taiwan's Database of Medicinal Plants (TCM) is currently the world's largest non-commercial database based on information collected from Chinese medical institutes and authoritative scientific journals. In the last decade, with the advent of new generation sequencing (NGS) technology, gene sequencing and diagnosis of genetic diseases have entered a new field. By using this technique, it has been possible to determine the genetic cause of many diseases and syndromes, including congenital disorders and abnormalities, which were previously described as "unknown causes" due to the limitations of the techniques used. In fact, NGS technology consists of a series of methods consisting of preliminary preparation and fragmentation of the studied genome sample, sequencing, imaging and visualization, assembling the sequenced parts and data analysis. Among the applications of this new method, we can mention a significant improvement in the diagnosis of genetic diseases, pre-implantation genetic diagnosis, pharmacogenomics, epigenetics and identification of structural variations in the genome. Given that colitis is one of the most common diseases in the country and the interest in using herbal medicines to cure intestinal inflammation is increasing day by day. In the present research, we aim to identify the number of target molecules in the innate immune system with a high difference by analyzing the transcriptome of these diseases and using the virtual screening technique to search for plant compounds that have antagonistic capabilities for these receptors. Also, by using this in vitro culture, check and confirm the anti-inflammatory properties of these compounds. The statistical community includes 200 human transcriptome runs, about 60 thousand compounds related to medicinal plants and in vitro experiments with at least three experimental replicates and three technical replicates. In this study, the anticancer and immunomodulatory effects of the aqueous extracts of rosemary and nettle medicinal plants were investigated as a promising source of cancer treatment against the AGS cell line derived from gastric cancer. IC50 of the extracts was determined by MTT assay. Flow cytometry and Real-Time PCR were used to measure apoptosis and evaluate the expression of some genes involved in cell signaling. The results of the MTT test for the effect of rosemary and nettle extracts separately and simultaneously on the survival percentage of AGS cell line derived from gastric cancer and the results showed that the highest amount of viable cells in the control and the lowest amount in the simultaneous combination of rosemary extract and Nettle and then nettle (100%) have been observed alone.

Keywords: cancer, nettle, rosemary, MTT, bioinformatics analysis