Med chem 2015, 5:10
http://dx.doi.org/10.4172/2161-0444.C1.016

OMICS International
conferenceseries.com

4th International Conference on
Medicinal Chemistry & Computer Aided Drug Designing
November 02-04, 2015 Atlanta, USA

In silico analysis for predicting fatty acids of black cumin oil as inhibitors of P-glycoprotein

Babar Ali[1, 2], **Qazi Mohd Sajid Jamal**[1], **Showkat R Mir**[2], **Saiba Shams**[3], **Mohd Rashid**[1], **Naser A Al-Wabel**[1] and **Mohamamd A Kamal**[4]
[1]Buraydah Colleges, Kingdom of Saudi Arabia
[2]Jamia Hamdard, India
[3]Siddhartha Institute of Pharmacy, India
[4]King Abdulaziz University, Kingdom of Saudi Arabia

Background: Black cumin oil is obtained from the seeds of *Nigella sativa L.* which belongs to family Ranunculaceae. Seeds oil has been reported to possess anti-tumour, antioxidant, antibacterial, anti-inflammatory, poglycaemic, central nervous system depressant, antioxidant and immuno-stimulatory activities. These bioactivities have been attributed to the fixed oil, volatile oil, or their components. Seed oil consisted of 15 saturated fatty acids (17%) and 17 unsaturated fatty acids (82.9%). Long chain fatty acids and medium chain fatty acids have been reported to increase oral bioavailability of peptides, antibiotics and other important therapeutic agents. In earlier study, permeation enhancement and bio-enhancement of drugs has been done with black cumin oil.

Objective: In order to recognize the mechanism of binding of fatty acids to P-gp, linoleic acid, oleic acid, margaric acid, cis-11, 14-eicosadienoic acid and stearic acid were selected for *in silico* studies which were carried out using AutoDock 4.2, based on the Lamarckian genetic algorithm principle.

Materials & Methods: Template search with Blast and HHBlits has been performed against the SWISS-MODEL template library (SMTL). The target sequence was searched with BLAST against the primary amino acid sequence of P-glycoprotein from *Rattus norvegicus.*

Results: The amount of energy needed by linoleic acid, oliec acid, eicosadeinoic acid, margaric acid and stearic acid to bind with P-gp was found to be -10.60, -10.48, -9.95, -11.92 and -10.37 kcal/mol, respectively. The obtained data supports that all the selected fatty acids have contributed to inhibit P-gp activity thereby enhance the bioavailability of drugs.

Conclusion: This study plays a significant role in finding hotspots in P-gp and may offer further scope of designing potent and specific inhibitors of P-gp.

babarasifpharma@gmail.com

Antioxidant activity and free radical scavenging properties of captopril

Akbar Hedayatizadeh-Omran
Mazandaran University of Medical Sciences, Iran

Several diseases are associated with oxidative stress caused by free radicals and reactive oxygen species. In this study, antioxidant activity of captopril was studied using *in vitro* assays systems. Free radical scavenging and reducing power were determined with Diphenyl Picryl Hydrazyl free radical (DPPH method) and potassium ferricyanide method, respectively. The results of this study showed that captopril possessed a significant free radical scavenging and reducing power properties and there was a clear correlation existing between antioxidant activity and concentration of captopril. Percentage of free radical scavenging of captopril was more than 92% at concentration 0.08 mM.

akbar_hedayati@yahoo.com

Notes: