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Research Article

STUDY OF DRUG LIKENESS ACTIVITY OF PHYTOCHEMICALS IN MEDICINAL PLANTS

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ABSTRACT
Phytochemicals in medicinal plants can deliver potential therapeutic drugs such as anticancer, antiviral, antioxidant etc. The plant kingdom is a treasure house of potential drugs and each phytochemical cannot be tested in the wetlab preparations. Hence the main aim of the study is the drug likeness activity of phytochemicals in medicinal plants such as *Anethum graveolens, Apium graveolens* against hepatocellular carcinoma. These plants have anticancer, antilivercancer, hepatoprotective, antiviral activities. Focusing on these activities, the phytochemicals from these plants were collected from Dr.Duke Phytochemical and ethnobotanical database. The drug likeness is evaluated by satisfying Lipinski's rule of five, ADMET properties, Partition coefficient analyzed through Accelerys Discovery studio. The results screen the phytochemicals and these interpretations can be further preceded for the drug designing.
Keywords: *Apium graveolens, Anethum graveolens,* ADMET.

INTRODUCTION

Anethum graveolens (dill) is an annual, erect, 50-150cm tall and glabrous herb belongs to family Apiaceae. Dill includes essential oils, fatty oil, moisture (8.39%), proteins (15.68%), carbohydrates (36%), fiber (14.80%), ash (9.8%) and mineral elements such as calcium, potassium, magnesium, phosphorous, sodium, vitamin A, and niacin. The major components of *Anethum graveolens* are flavonoids, phenolic compounds and essential oil[1,2]. A. graveolens exhibited significant anti-stress, antioxidant[3], antibacterial[4], cardio protective agent[5].

Apium graveolens is a biennial with stems 0.3-2.4 m, were erect and branching belonging to the family Apiaceae[4]. .*Apium graveolens* (Celery) is rich in beta-carotene, folic acid, vitamin C, magnesium, potassium, silica, sodium, chlorophyll and fiber. It contains 95% water[6]. The major components of *Apium graveolens* are alkaloids, glycosides, terpenoids, flavonoids, tannin, polyphenols[7, 8]. The plant has antimicrobial[10], anticancer [8], hepatoprotective activity [11].

The present study is to screen the phytochemical in these medicinal plants which show both anticancer and antiviral activity against hepatocellular carcinoma to deliver a best drug compound.

MATERIALS AND METHODS

Dr. Duke's Phytochemical and Ethnobotanical database

These databases contain information on the activity of chemicals in plants, and ethanobotanical uses for plants. Databases are searchable by plant (scientific or common name), chemical (e.g., ascorbic acid), or activity (e.g., antiviral)

Chemspider

ChemSpider is a free chemical structure database providing fast text and structure search access to over 28 million structures from hundreds of data sources.

Accelerys Discovery Studio

Accelerys Discovery Studio software provides comprehensive modeling and simulation capabilities for computational chemists, computational biologists, and other scientists engaged in small molecule and biotherapeutics-based research.

Accelerys-Admet

Open the prepared ligand and then click protocol ADMET, then select ADMET distributors and then run the program. After job completed double click on it and view the results. If the ligand is natural compound open the prepared ligand, then click protocol ADMET and then select – ADMET TOPKAT (Toxicity Prediction by Komputer Assisted Technology). Choose the models, Change the detailed report as true and then run the program. After job completed double click on it and view the results in pdf form.

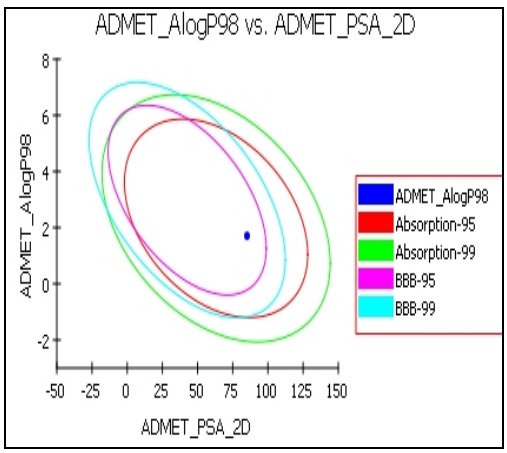

Figure 1: Admet of satisfied phytochemicals

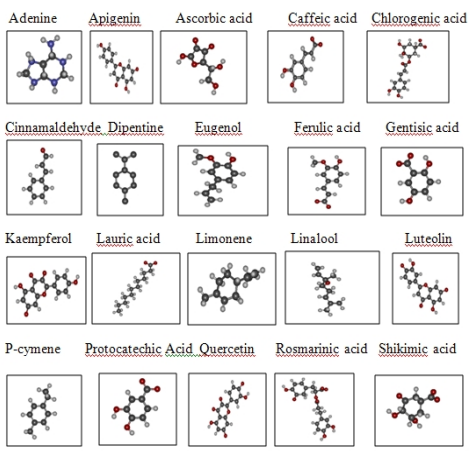

Figure 2: Structures of concluded phytochemicals

RESULTS AND DISCUSSION

Phytochemicals in *Anethum graveolens*

Phytochemicals showing anti cancer activity are Alpha Terpineol, Alpha Tocopherol, Caffeicacid, Hyperoside, Isoquercitrin, Kaempferol, Limonene, Rutin. Phytochemicals showing antilivercancer are chlorogenic acid and Ferulic acid. Phytochemicals showing antiviral are Alpha-pinene, Apigenin, Ascorbic acid, Beta-sitosterol, Caffeicacid, Chlorogenic acid, Dipentine, Ergosterol, Eugenol Ferulic acid, Hyperoside, Kaempferol, Lauric acid, Limonene, Linalool, Luteolin-7-Glucoside, P-Cymene, Quercetin, Quercitrin, Rosmarinicacid, Rutin, Stigmasterol.

Phytochemicals in *Apium graveolens*

Phytochemicals showing anticancer activity are Alpha terpineol, Alpha tocopherol, Beta-carotene, Caffeicacid, Isoquercitrin, Kaempferol, Limonene, Rutin, Shikimic acid. Phytochemicals showing antilivercancer are Chlorogenic acid and Ferulic acid. Phytochemicals showing antiviral are 8-methoxy-psoralen, Adenine, Alpha-pinene, Angelicin, Apigenin, Ascorbic acid, Beta-sitosterol, Caffeic acid, Chlorogenic acid, Cinnamaldehyde, Eugenol, Ferulic acid, Formaldehyde, Gentisic acid, Kaempferol, Lauric acid, Limonene, Linalool, Luteolin, Neryl-acetate, P-Cymene, Protocatechuic acid, Psoralen, Quercetin, Rutin, Stigmasterol.

Failed compounds in both plants

Alpha-Terpineol, Alpha-tocopherol, Hyperoside, Isoquercitrin, Rutin, Alphapinene, Ergosterol, Beta-sitosterol, Lutoelin-7-Glucoside, Quercetin, Stigmasterol, 8-methoxy-psoralen, Alpha-pinene, Formaldehyde, Neryl acetate.

DISCUSSION

In ***Anethum graveolens*** 32 phytochemicals were selected and in ***Apium graveolens*** 37 compounds were selected. In both the plants there were repeated phytochemicals showing anticancer, antiviral, antilivercancer activity. Hence in grand total, 16 compounds failed to satisfy Lipinsky's rule of five due to Hydrogen bond acceptor>10, Partition Coefficient>5, Molecular weight>500. In total 21(table1) compounds satisfied the ADMET properties(fig 1) of Blood brain barrier and Plasma protein binding to be above 95%, Hepatotoxicity to be zero, CYPD26 inhibition, AlogP to be less than 5 and the structures are shown in the figure 2. Hence these compounds can be further proceeded for docking studies to design a best drug compound and then to a wet lab preparations.

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