



Structure Based Analysis of Tumor Inducing NF- κ B Protein Using Phytochemical from *Catharanthus Roseus* Medicinal Plant

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Abstract

NF- κ B plays important role in inflammatory response. Hence, the method of inhibiting NF- κ B signaling has potential therapeutic application in cancer and inflammatory diseases. Conventional drug vinpocetine is used for treatment of cancer. The other conventional drug (vindoline, vindolinine, catharoseumine) are used for diabetes, curing hypoglycemic effects, curing hypertension and cancer too. The present study is explore vindoline, vindolinine and catharoseumine in comparison to vinpocetine by using molecular docking. The online server 'swiss ADME analysis' detected the physiochemical pharmacokinetics and drug likeness score and medicinal chemistry of vinpocetine and conventional drugs. Results from swiss ADME analysis showed that vinpocetine and conventional drugs did not violate the "Lipinski five rule" for drug. The resulted binding energy of vindoline, vindolinine and catharoseumine were -6.5, -8.17 and -8.6 respectively. The binding energy (-8.6 kcal/mol) of catharoseumine was higher than vinpocetine (-7.35 kcal/mol). Thus, catharoseumine has greater potential to interact with interacting residues of NF- κ B further consideration as an anti cancerous regimen.

Keywords: Tumor; NF- κ B Protein; Phytochemical; *Catharanthus Roseus*; Medicinal Plant

Introduction

Catharanthus roseus is native to Indian Ocean island of Madagascar. *Catharanthus roseus* L (Madagascar periwinkle) have several synonyms like, *Vinca rosea*, *Ammocallis rosea* and *Lochnera rosea*. Others English names occasionally used for the plant include Cape periwinkle, Rose periwinkle, Rosy periwinkle and Old maid. It is an medicinal plant containing alkaloids, used in diabetes, blood pressure, asthma, constipation, cancer and menstrual problem. The periwinkle logo as a symbol used for hope for cancer patients which is used by National Cancer council of Malaysia. Stem produces a milky sap which is source for more than 70 indole alkaloids. Vincristine and vinblastine are the alkaloids were isolated from this plant are well known anti-cancer drugs for Hodgkin's lymphoma and childhood leukemia respectively. But, there are some major side effects of these drugs are hair loss, peripheral neuropathy, constipation and hyponatremia. The plant has a long

history of using Ayurvedic medicine, traditional Chinese medicine and other healing systems [1].

Scientific Classification

Kingdom: Plantae

Division: Magnoliophyta (Flowering plant)

Class: Magnoliopsida (Dicotyledone)

Order: Gentianales

Family: Apocynaceae

Genus: *Catharanthus*

Species: *roseus*

Geographical distribution

Catharanthus roseus is native to the Indian Ocean island of Madagascar. It commercially cultivated in Spain, US, China, Africa, Australia, India and Southern Europe for its medicinal uses. It is now