

Assessment of dual inhibitory activity of epifriedelanol isolated from *Cayratia trifolia* against ovarian cancer

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Abstract

Cayratia trifolia is used as diuretic, in tumors, neuralgia and splenopathy. However, compounds depicting anti-ovarian cancer activities from this plant source have not yet been identified and structurally characterized till date. In the present study, X-ray structure of epifriedelanol, a bioactive compound, isolated from the ethanolic extract of the *C. trifolia* and its binding affinities against a few proteins (HER2, EGFR and CXCR4) that are reported to get overexpressed under ovarian cancer had been thoroughly studied by using molecular docking means. Binding affinities of the compound vis-à-vis that of carboplatin, a FDA approved drug to the ovarian cancer, to interact with the protein targets are quite impressive. The drug-likeness properties of the epifriedelanol and scope to develop the compound as a potent anti-ovarian cancer drug are discussed in this paper.

Introduction

Ovarian cancer accounts for the highest tumor related mortality among gynecologic malignancies and is the fifth most frequent cause of cancer related death. In 2014, the incidence rate for women in developed countries was about 9.4 per 100,000 compared to 5.0 per 100,000 in developing countries. However, approximately 25% of cases are diagnosed between ages 35 and 54 (Jayson et al., 2014). Above 70% of women were diagnosed with late stage III and IV disease.

Although not withstanding great advancements have been made in the treatments and management control of the cancer progression. A number of undesired adverse effects, sometimes, occurs during chemotherapy (Desai et al., 2008). Research reports suggest that compounds from natural sources are superior to synthetic compounds in terms of pharmacokinetic and pharmacodynamics properties.

In general, usage of medicinal compounds is always superior to the synthetic compounds. So, the recent research has been focused towards the plant compound isolation and compounds production at large scale (Fortes et al., 2012).

A large proportion of the World population depends on the traditional medicine because of the shortage and high expenses of orthodox medicine (Dutta and Maharia, 2012; Li et al., 2011; Sultana et al., 2011). Natural products play a central role in the development of novel drug for the treatment and prevention of diseases (Khan et al., 2015; Sharma et al., 2015; Yu et al., 2013; Dhanamani et al., 2011).

Cayratia trifolia (L.) is commonly known as Fox grape in English, Kattuppirantai in Tamil, Amlabel and Ramchana in Hindi and Amlavetash in Sanskrit (Perumal et al., 2014; Perumal et al., 2015). It has been reported to contain huge amount of bioactive compounds such as