

Chapter 12

ADMET Prediction and Molecular Simulation of Desmostachya bipinnata Against Gastric Cancer Protein (PFN1)

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ABSTRACT

Being the fourth most prevalent cancer and the second main cause of cancer death globally, gastric cancer is a serious health issue. Despite significant improvements in our knowledge of epidemiology, pathology, molecular causes, and therapeutic options and tactics, as well as a drop in incidence and death, the burden of disease remains high. This work involves development of potential anti-cancer drug from the bioactive compounds of Desmostachya bipinnata, an invasive shrub which is found in all over the state of Tamil Nadu. The compounds of Desmostachya bipinnata were screened for ADMET properties and docked against the profilin-1 (PDB: 4x1l). The protein-ligand complex which formed due to molecular docking, stigmasterol-PFN1 with least binding affinity of -7.34 Kcal/mol is chosen for simulation studies. Dynamics simulation is used to model the firmness and stability of protein-ligand complex. CHARM-GUI and NAMD software is used for dynamic simulation studies for this work.

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1. INTRODUCTION

1.1 Overview of Gastric Cancer

Gastric cancer, often known as stomach cancer, is a fatal condition that develops in the stomach's inner lining. It is a complicated disease with numerous components that are influenced by a combination of genetic, environmental, and lifestyle factors, making it a serious worldwide health issue (Plummer et al, 2016). Gastric cancer, which has diverse incidence rates around the world, continues to be a major cause of cancer-related morbidity and mortality. Due to its frequent asymptomatic or nonspecific clinical presentation in its early stages, gastric cancer poses significant problems in early identification and management (Thrift et al, 2020). The condition can advance in stages, starting with chronic gastritis and ending with invasive cancer after moving through atrophic gastritis, intestinal metaplasia, and dysplasia. The continuous infection of the stomach lining with *Helicobacter pylori*, a bacterium known as a key risk factor and a prominent driver of gastric carcinogenesis, is essential to the development of gastric cancer (Subsomwong et al, 2017).

The number of cases of gastric cancer varies significantly by region, with greater rates being seen in East Asia, Central and South America, and some sections of Eastern Europe. According to the World Cancer Research Fund, there were over 770,000 fatalities and close to 1.1 million new cases of stomach cancer worldwide in 2018. These figures demonstrate the disease's significant impact on public health and the urgent need for efficient preventive and therapeutic measures (Benbrahim et al, 2017).

1.2 Plant Source (*Desmostachya bipinnata*)

Perennial grass *Desmostachya bipinnata* Linn, a member of the Graminae family, is found in large quantities throughout India. In the traditional medical system of India, the roots and leaves are utilized. Reference literature has documented the usage of kush as medicine and its numerous therapeutic benefits. Kush is described in Ayurveda as being acrid, cooling, oleaginous, aphrodisiac, diuretic, and helpful in treating blood disorders, biliousness, asthma (Dama), thirst, strangury, jaundice, vaginal discharge, vesical calculi, ailments of the skin, bladder, and uterine, among other conditions (Vivekanandarajah et al, 2021). Rootstock that has been powdered is used as an astringent, galactagogues, and diuretic.

1.3 Role of PFN1 Protein in Gastric Cancer

Over thirty years ago, profilin-1 (PFN1), a critical actin-binding protein, was found in the calf thymus. PFN1 has recently been shown to play a biological role in cancer. Almost all cellular functions, including gene transcription, endocytosis, motility, proliferation, and survival, depend on this protein. PFN1 is underexpressed in a variety of human solid tumors, including carcinomas of the liver, pancreatic, and breast (Huang et al, 2020). However, overexpression of this protein can stop these cancer cells from multiplying and migrating, suggesting that PFN1 may have tumor-suppressive properties. On the other hand, PFN1 overexpression in tumors other than lung and kidney malignancies, like laryngeal and renal cell carcinoma, has been demonstrated in numerous investigations. Due to these variations, PFN1 may have a role in many tumorigenic processes (Wang et al, 2021).

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