Chapter 11
ADMET Prediction and Molecular Simulation of Prosopis juliflora Against Lung Cancer Protein (ATK1)

Arun Pandiyan S.
Vels Institute of Science, Technology, and Advanced Studies, India

Vivek Pazhamalai
Vels Institute of Science, Technology, and Advanced Studies, India

V. Gokul
Vels Institute of Science, Technology, and Advanced Studies, India

Ivo Romauld S.
Vels Institute of Science, Technology, and Advanced Studies, India

L. Madhumitha
Vels Institute of Science, Technology, and Advanced Studies, India

S. S. Meenambiga
https://orcid.org/0000-0002-5445-525X
Vels Institute of Science, Technology, and Advanced Studies, India

ABSTRACT

With 85% of cases being non-small-cell lung cancer (NSCLC), it is the most prevalent form of the disease. NSCLC normally develops and spreads more slowly than its counterpart, small-cell lung cancer (SCLC), which may result in a worse outcome. Adenocarcinoma, squamous cell carcinoma, and giant cell carcinoma are only a few of the subtypes of NSCLC. Each has distinct traits and approaches to treatment. Smoking continues to be a substantial risk factor for NSCLC, although it can also afflict non-smokers. This work involves development of potential anti-cancer drug from the bioactive compounds of Prosopis juliflora, an invasive shrub which is found in all over the state of Tamil Nadu. The bioactive compounds of Prosopis juliflora were screened for ADMET properties and docked against the RAC-alpha serine/threonine-protein kinase (PDB: 3o96). Then, the compound Phenol, 3,5-bis(1,1-dimethylethyl)- which has the least binding energy of -6.95 kcal/mol was used to model the firmness and dynamics of the free protein 10 picoseconds.

DOI: 10.4018/979-8-3693-1646-7.ch011

1. INTRODUCTION

1.1 Overview of Lung Cancer

Lung cancer is a malignancy characterized by the uncontrolled growth of neoplastic cells in the lung tissues. It is a heterogeneous disease with two predominant histological subtypes: non-small cell lung cancer (NSCLC), which comprises approximately 85% of all cases, and small cell lung cancer (SCLC), a more aggressive but less common variant (Schabath et al, 2019). The primary etiological factor associated with lung cancer is tobacco smoking, accounting for a substantial portion of cases. Additional risk factors include exposure to environmental carcinogens, genetic predisposition, and other occupational hazards. Lung cancer often remains clinically silent until it reaches advanced stages, at which point patients may exhibit a constellation of symptoms, including chronic cough, hemoptysis, chest pain, dyspnea, and unintentional weight loss (Travis, 2012).

Lung cancer is the leading cause of cancer-related deaths globally in both men and women, with a 14% five-year survival rate despite advancements in diagnostic techniques, and the majority of patients still present with severe disease (Bunn, 2012). Over half of lung cancer cases have no cure at diagnosis, and Stage I patients have remarkably low survival rates. Understanding molecular changes linked to poor prognosis is crucial for improving diagnosis and patient care. Genomics and proteomics have been developed to study genes and proteins in specific cell or tissue types. Differential profiling can help identify differences between tumors and normal tissues in cancer. Gene and protein expression patterns can improve lung cancer treatment by enhancing categorization and diagnostic classifiers (Gadgeel et al, 2012).

Lung cancer metastasis occurs when cancerous cells break away from the primary tumor in the lungs and enter the bloodstream or lymphatic system. These cells can travel to distant organs and tissues, where they establish new cancerous growths. The propensity of lung cancer to metastasize is attributed to several factors, including the highly vascularized nature of the lungs, which allows cancer cells to easily access the bloodstream, and the ability of lung cancer cells to evade the body's immune system (Popper, 2016). Common sites for metastasis in lung cancer include the brain, bones, liver, and adrenal glands. The brain is a frequent site due to its proximity to the lungs and the interconnected blood supply. Bone metastases can cause pain and fractures. Liver metastases can lead to impaired liver function, while adrenal gland involvement can disrupt hormone production (Riihimäki et al, 2014).

1.2 *Prosopis Juliflora*

Prosopis juliflora, an invasive plant species, is expanding rapidly in tropical and subtropical regions. As a resilient xerophyte, it provides shelter, reduces erosion, enhances micrometeorology, and provides food, feed, fuel, medicines, and cosmetics to the poor. Introduced in areas with less harsh climates and greater soil and water availability than existed in its natural environment as a result of attempts undertaken during the 19th and 20th centuries to capitalize on these characteristics of *P. juliflora* (Patnaik et al, 2017). In vitro pharmacological activities of *P. Juliflora* seed and leaf extracts include antibacterial, antifungal, and anti-inflammatory characteristics. P. juliflora is a popular traditional medicine remedy for treating inflammation, flu, sore throat, cold, measles, excrescences, dysentery, diarrhea, and wound healing. As a whole, Prosopis is known as kalpataru in India, which refers to "wonder tree" and "king of the desert," as all of the tree's parts are therapeutic (Ukande et al, 2019).