

Chapter 14

Understanding Pharmacokinetics, Bioavailability Radar, and Molecular Docking Studies for Selected Medicinal Plants Against Lung Cancer Receptors

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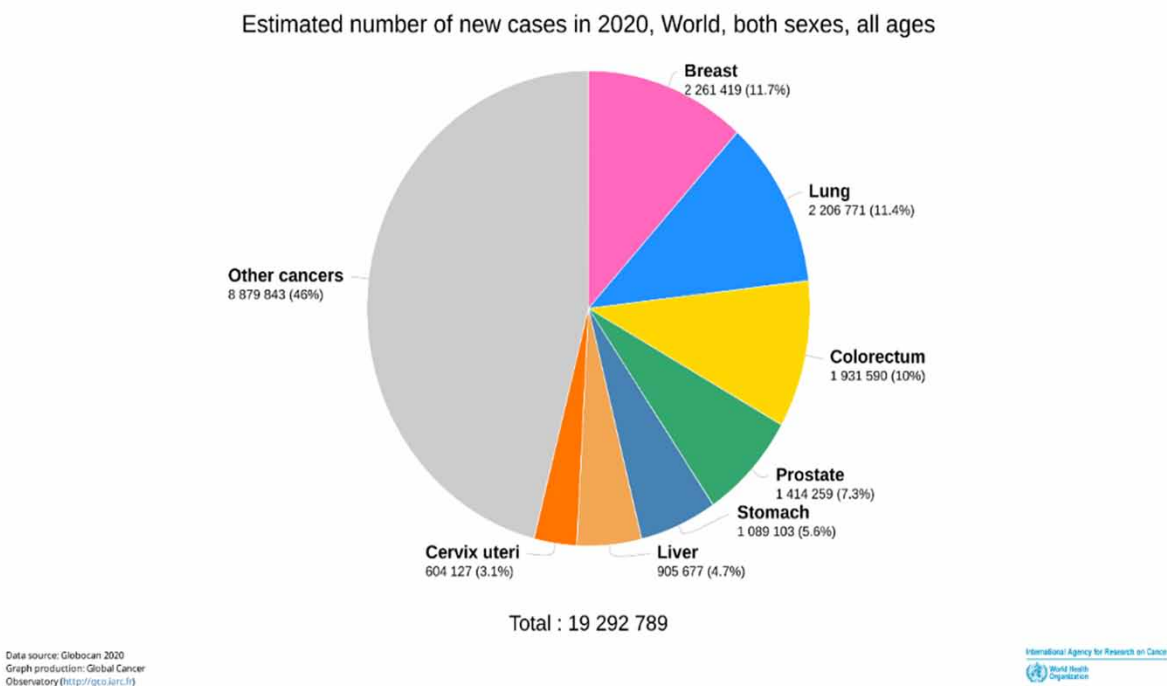
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ABSTRACT

This chapter is dedicated to discussing molecular docking approaches in natural product-based drug discovery programs, which include 27 phytochemicals from 11 distinct medicinal plants. The ADME (absorption, distribution, metabolism, excretion) processes are first examined to understand how a drug interacts within and is processed by the body. Acquiring knowledge about a drug's ADME properties is vital to developing safe and effective pharmacotherapy. A Bioavailability radar analysis is then conducted to identify the optimal physicochemical space required for a molecule to be classified as drug-like, which includes polarity, size, lipophilicity, solubility, flexibility, and saturation. Molecular docking is a useful method in traditional medicine screening programs that predicts interactions between small molecules and drug targets. Finally, the target protein is selected for the study, which is optimized with the coordinates of the phytochemicals for stable conformation and minimum energy.

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Figure 1. Estimated Cancer Cases
Siegel et al. (2023)



INTRODUCTION

Cancer occurs when irregular cells develop uncontrollably and spread beyond their normal outlines to adjacent parts of the body and other organs. Cancer cells can develop in almost any tissue or organ in the body as well as cause many diseases (Sung et al., 2021). Approximately, 9.6 million people died from cancer in 2020, making cancer the second most common cause of death worldwide. Men are most frequently affected by lung, liver, stomach, prostate, and colorectal cancer, while breast, lung, thyroid, colorectal and cervical cancer are the most frequent types surrounded by women (Inamura, 2017).

The most common cause of cancer death was lung cancer, causing around 1.8 million deaths (18% of all deaths caused by cancer). Colorectal cancer is the second leading common cause of death caused by cancer, accounting for 9.4% of all deaths caused by cancer, followed by liver cancer (8.3%), stomach cancer (7.7%), and female breast cancer (6.9%) (Siegel et al., 2023).

Treatment of cancer has been the biggest challenge for society. Several ways have been seen for the treatment of cancer which consist of:

- Surgery: It is performed with the objective of removing cancer or as much of it as attainable (Sullivan et al., 2015).
- Chemotherapy: Drugs are used in chemotherapy to kill cancer cells (Agarwal, 2016; Bashir, 2023).
- Radiation therapy: High-powered energy beams, such as protons or X-rays are used to destroy cancer cells (Shaz, 2019).

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