

ABSTRACT

LAILA FITRIANY. 2025. *An In Silico Study on the Anticancer Potential of Compounds from Mimosa pudica L. as a Candidate for Lung Cancer Treatment and a Biology Learning Resource*. Biology Education Department, Faculty of Science and Teacher's Training, Siliwangi University of Tasikmalaya.

Mimosa pudica L. is a tropical plant known to contain various bioactive compounds such as flavonoids, alkaloids, and triterpenoids, which have been widely used in traditional medicine. One of its therapeutic potentials is as an anticancer agent. Lung cancer is among the leading causes of death worldwide, thus necessitating safer and more affordable alternative treatments. This study aims to explore the potential compounds of Mimosa pudica L. as a candidate for lung cancer therapy through an in silico approach, and to develop biology learning resources based on the research findings. The methods used include molecular docking, molecular dynamics simulations, as well as pharmacokinetic and toxicity predictions. The selected target protein was EGFR (PDB ID: 3W33). The docking results showed that stigmasterol had the highest affinity with a rerank score of -12.44. The 100-ns molecular dynamics simulation indicated that the stigmasterol–EGFR complex was stable, with RMSD values ranging from 1.4 to 4.3 Å and low RMSF values at active site residues. This compound also met the criteria of Lipinski's Rule of Five, showed favorable ADMET profiles, and had a toxicity level of 4 (categorized as low). This research produced a scientific article and a booklet as contextual learning resources integrating bioinformatics technology and local potential. Thus, Mimosa pudica L. has promising potential as a candidate for lung cancer therapy and as an innovative biology learning material.

Keywords: anticancer, biology learning resources, EGFR, in silico, Mimosa pudica L.