Pharmacological Studies, Isolation and Structure Identification, and Investigation of the Mechanism of Molecular Action of Bioactive Compounds from Bajakah Plants (Spatholobus littoralis Hassk) Typical of Kalimantan as Anti-Cancer

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ABSTRACT

Introduction: *Spatholobus littoralis* is widely used as an anticancer herbal medicine in Kalimantan, Indonesia. This study aims to determine the cytotoxic effect of *S.littoralis* on breast cancer cells in vitro and predict the mechanism of its activity on the estrogen receptor (ER) in silico.
Method: Dry wood of *S. littoralis* was extracted using ethanol solvent by maceration and fractionated using *n*-hexane, chloroform, and ethyl acetate. The cytotoxic assay was evaluated using MTT reagent in T47D and 4T1 cells. Prediction of the interaction mechanism of phenolic compounds from the genus *Spatholobus* with ER-α and ER-β was carried out in silico.
Result: The results showed that the ethanolic extract of *S. littoralis* did not show a cytotoxic effect on T47D cells, but showed weak toxicity on 4T1 cells. Furthermore, each *n*-hexane, chloroform, and ethyl acetate fraction of *S. littoralis* showed strong to moderate cytotoxic effects on T47D and 4T1 cells. In silico test results showed that 3'-4'-7-trihydroxy flavone was a phenolic compound with the highest binding energy compared to the ER native ligand Genistein in ER-α (-10.2 Kcal/mol) and ER-β (-10.9 Kcal/mol). The 3'-4'-7-trihydroxy flavone binding site in ER-α was bound to amino acid residues Arg394, Glu353, and Leu387, while in ER-β it was found at Arg346, Glu305, and Leu339.
Conclusion: These findings indicate that *S. littoralis* contains phenolic compounds that can inhibit the growth of breast cancer cells, so it has the potential to be developed as a new drug for breast cancer.

Kata Kunci: *Spatholobus littoralis, Cytotoxic effect, Breast cancer, Estrogen receptor, In silico*