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Research Article

# Untargeted UHPLC-Q exactive orbitrap HRMS-based network pharmacology for the discovery of anti-breast cancer compounds from *spatholobus littoralis* stems fractions and experimental validation

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## Abstract

*Spatholobus littoralis* has been traditionally used by the Dayak tribe as a medicine to treat breast cancer. However, its bioactive components and mechanisms of action remain unclear. To identify the bioactive compounds in the aqueous fraction of the 70% ethanol extract of *S. littoralis* stems and elucidate their mechanisms of action as an anti-breast cancer agent. The fractions of the 70% ethanol extract were tested for antioxidant activity and aqueous fraction was analysed for bioactive compounds by using UHPLC-Q-Orbitrap-HRMS, network pharmacology, molecular docking, and experimental validation. The protein-protein interaction (PPI) analysis identified 10 target genes related to breast cancer, with KEGG pathway analysis indicating activity in breast cancer. The molecular docking analysis showed binding affinities from  $-5.7$  to  $-7.5$  kcal/mol. The experimental validation using cytotoxicity testing resulted in an  $IC_{50}$  value of  $121.66 \mu\text{g/mL}$ . Several bioactive compounds from the aqueous fraction exhibited anti-breast cancer activity *via* EGFR tyrosine kinase inhibition.

## Graphical Abstract

