

***In vitro* cytotoxicity of *Clinacanthus nutans* fractions on breast cancer cells and molecular docking study of sulphur containing compounds against caspase-3**

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ABSTRACT

Clinacanthus nutans has attracted Malaysian public interest due to its high medicinal value in the prevention of cancer. Currently, the specific compound or compounds giving rise to the anticancer potential of *C. nutans* has not been investigated thoroughly. The extraction was carried out by MeOH at room temperature using the powdered bark of *C. nutans*, while chromatography was carried out on a silica gel RP-18 column using the crude methanolic extract. Six fractions collected from column chromatography were evaluated by MTT assay against two breast cancer cell lines: MDA-MB-231 and MCF-7. Amongst the fractions, A12 and A17 were shown to exhibit the highest activity. Two sulphur-containing compounds, viz., entadamide C (1) and clinamide D (2), were isolated from these fractions. Molecular docking simulation studies revealed that entadamide C and clinamide D could bind favourably to the caspase-3 binding site with the binding energy of -4.28 kcal/mol and -4.84 kcal/mol, respectively. This study provides empirical evidence for the presence of sulphur-containing compounds in the leaves of *C. nutans* that displayed anticancer effects which explains its ethnomedicinal application against breast cancer. The docking simulation study showed that both compounds could serve as important templates for future drug design and development.

KEYWORDS

Clinacanthus nutans; Cytotoxicity; MDA-MB-231; MCF-7; Sulphur containing compounds; Molecular docking; Caspase-3

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