from the Brazilian tarantula spider named *Acanthoscurria gomesiana* with potential cytotoxicity against cancer cells. This study used computational techniques for the interpretation of peptide-protein interactions between the Gomesin peptide and suitable target protein. The AKT1 protein, a significant activator in cancer cell growth signaling was identified as the selected target protein with the PharmMapper server. The homology structure of the Gomesin peptide was obtained using the Protein Data Bank (PDB) web server of the RCSB server, and the homology modelling of AKT1 protein was conducted via CHARMM-Gui web server from the UniProt database. The interaction was determined using molecular docking via HADDOCK (High Ambiguity Driven DOCKing), which provided evidence that during Peptide-protein complex production the specific binding areas are expected to inhibit through allosteric inhibition. At the end of this study, the dynamic motion behavior of the Gomesin-AKT1 complex applied for 100ns with CHARMM GUI web server, proved to have more affinity and stability towards disrupting the activation of the selected cancer growth signals.

Keywords:
Anticancer peptide, AKT1, Molecular docking, MD simulation, Cancer drug

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Evaluation of the anti-inflammatory activity and bioactive compounds of *Citrus aurantifolia*(L) leaf extracts

D. Jagoda[1,2], G.D Liyanaarachchi[1], H.D Weeratunge[1], Shiroma M. Handunnetti[2], Narmada Fernando[2], J.K.R.R. Samarasekara[1]*

[1] *Industrial Technology Institute. Colombo 7.*

[2] *Institute of Biochemistry, Molecular Biology and Biotechnology, University of Colombo, Colombo 3.*

**Corresponding author: radhika@iti.lk*

Citrus aurantifolia L. is used in traditional systems of medicine as remedy for stomach ailments, constipation, headache, arthritis, colds, coughs, sore throats, and appetite stimulant. This study investigated the chemical composition and the immunomodulatory activity of the ethanolic extract and essential oils extracted by Hydro distillation (HD) from the leaves of *Citrus aurantifolia* L. The bioactivities were evaluated by performing DPPH free radical scavenging assay, ferric ion reducing antioxidant power (FRAP) assay, 5-lipoxygenase inhibition (5-LOX) assay, inhibition of LPS-induced Nitric Oxide (NO) production by Griess assay, total phenolic content (TPC) and total flavonoid content (TFC). The EO was analyzed for its chemical compositions using Gas Chromatography-Mass Spectrometry (GC-MS) to identify the chemical components for bioactivity. The ethanolic extract of *C. aurantifolia* leaves were given the IC_{50} value of 735.29 ± 38.01 µg/ml for DPPH free radical scavenging assay. FRAP, TPC and TFC values for the ethanolic extract were 13.35 ± 2.09 µg/ml Trolox equivalent (TE)/g, 16.41 ± 1.59 mg Gallic acid equivalent (GAE)/g and 21.28 ± 0.42 mg Quercetin equivalent (QE)/g respectively. *C. aurantifolia* leaves ethanolic extract and EOs dose dependently inhibit 5-lipoxyganase enzyme having the IC_{50} values of 6.77± 0.34 µg/ml and 7.40 ± 1.46 µg/ml respectively, compared to the positive control baicalein IC_{50} value 1.76± 0.15 µg/ml. The percentage inhibition of NO production by LPS stimulated RAW 264.7 cells were 79% and 64% respectively for 250 µg/ml ethanolic extract and EO. A total of 87 phytochemicals were identified from *C. aurantifolia* leaves EO. D-limonene (35.65%) and Caryophyllene (20.91%) were major compounds and ϒ-elemene (3.93%), Caryophyllene oxide (3.62%), β-Bisabolene (3.11%), β-elemene (3.04%), are high in abundance. The result of ethanolic extract and EO showed appreciable reduction in nitric oxide production of LPS-stimulated RAW 264.7 cells and the inhibition of 5-LOX. Biologically active components in *C. aurantifolia* leaves are active against inflammation supports the ethnomedicinal claims of the use of the plant in the management of pain and inflammation.

Keywords:
Hydro-distillation, Gas Chromatography, Mass Spectrometry, Lipoxygenases, Griess assay.

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