

It is thus concluded that the polyaniline-cinnamon oil composite material act as a strong corrosion inhibitor of mild steel in aqueous HCl medium.

**Keywords:**

Mild steel, Polyaniline-cinnamon oil composite, Corrosion inhibition, Tafel plot, Electrochemical Impedance Spectroscopy (EIS), Scanning Electron Microscopy (SEM)

Abstract No: 2023\_23

## Production of biodiesel using waste cooking oil and loose copra oil

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This study focuses on producing biodiesel from waste cooking oil (WCO) and loose copra oil (LCO). The aim is to reduce energy consumption by using low-cost raw materials and energy-saving methods. With the global energy crisis, it is essential to find a sustainable alternative fuel source that is economical, easily transportable and environmentally friendly. Biodiesel has become a popular alternative to fossil fuels, but its production has drawbacks, including high energy consumption, longer production times, and high raw material costs. This study aims to address these drawbacks by using low-cost raw materials and energy-saving methods. Isopropanol (10% w/w) was used as a co-solvent to reduce energy consumption during the transesterification process and NaOH (1 wt%) was used as the catalyst. The quality of the biodiesel produced was determined by examining the fatty acid profile and specific fuel properties. The study

found that both WCO and LCO can be used to produce biodiesel. Under the best conditions (oil: CH<sub>3</sub>OH- 1:6 molar ratio, reaction temperature- 60 °C, stirring rate- 750 rpm, reaction time- 90 minutes), the maximum biodiesel yields obtained for WCO and LCO were 88.50% w/w and 90.60% w/w, respectively under addition of 10% w/w isopropanol. The specific fuel properties such as density, kinematic viscosity, and flash point of both WCO and LCO were comparable to ASTM limits, indicating their potential as alternative fuels. This study provides a potential solution to the energy crisis by producing biodiesel from low-cost raw materials and energy-saving methods, which has the potential to be a more sustainable and environmentally friendly alternative to fossil fuels.

**Keywords:**

Energy crisis, Biodiesel, Trans-esterification, Waste cooking oil, Catalyst

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## A Computational Approach to Determine the Potential Inhibition of the Gomesin Peptide as an AKT1 Inhibitor in Breast Cancer

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Animal trials and *in vitro* drug screening can improve drug discovery. However, such pre-clinical screenings are often costly and time-consuming. Due to this, a more effective technique is developed using *in silico* method for the same. Drug repositioning using multi-omics data represents a more effective approach over traditional drug development for new cancer-fighting therapies. In this study peptide-based drugs are identified

as an excellent candidate due to their properties, such as different amino acid charges, various sizes, polarity, and non-polarity characteristics, producing a composition against microbes and tumor cells. The peptides with anticancer activity, known as anticancer peptides (ACP), are biocompatible and provide a higher degree of specificity and selectivity between cancer and cancer-free cells. Gomesin is a natural antimicrobial peptide (AMP)

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

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*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<sub>50</sub> 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-lipoxygenase enzyme having the

IC<sub>50</sub> values of 6.77 ± 0.34 µg/ml and 7.40 ± 1.46 µg/ml respectively, compared to the positive control baicalein IC<sub>50</sub> 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  $\gamma$ -elemene (3.93%), Caryophyllene oxide (3.62%),  $\beta$ -Bisabolene (3.11%),  $\beta$ -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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