RESEARCH PAPER

# Structural and Pharmacological Evaluation of Momordica Phytochemicals: Linking Molecular Docking Affinities to in Vitro Cytotoxicity in Mcf-7 Breast Cancer Cells

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**ABSTRACT**

This study investigates the phytochemical profile and anticancer potential of Momordica species, particularly M. charantia. Utilizing an integrated approach of phytochemical profiling, molecular docking, and in vitro assays, the research identifies key bioactive leads. Methanolic extracts, especially from leaves, demonstrated significant antioxidant and cytotoxic activities. Molecular docking revealed high binding affinities for compounds like Cucurbitacin E and Momordicoside-G against cancer targets such as PI3K and Bcl-2. The findings suggest that Momordica phytochemicals serve as promising multi-target candidates for cancer chemoprevention and therapy.

**Introduction:** Cancer remains a leading cause of global morbidity, with approximately 20 million new cases and 9.7 million deaths reported in 2022. The rising burden is particularly acute in developing countries, necessitating low-cost, accessible interventions. Natural products have historically provided essential anticancer scaffolds, including taxanes and vinca alkaloids. The genus Momordica (Cucurbitaceae) is rich in bioactive secondary metabolites such as cucurbitane-type triterpenoids, phenolics, and flavonoids. Chronic oxidative stress, driven by reactive oxygen species (ROS), is a known contributor to mutagenesis and carcinogenesis. Phytochemicals from Momordica species may mitigate this through free radical scavenging and modulation of oncogenic signalling pathways like NF-κB and MAPK/ERK. This study aims to fill the research gap by providing a systematic structural and biological evaluation of these compounds.

**Materials and Methods:** Extraction was performed using various solvents, with methanol providing the highest yield of polar phenolics and triterpenoids. Phytochemical screening was conducted to identify major groups including saponins and flavonoids. In silico molecular docking was employed to predict the binding modes and interaction affinities between identified phytochemicals and cancer-associated protein targets. In vitro efficacy was evaluated through DPPH radical scavenging assays for antioxidant potential and MTT assays for cytotoxicity against breast cancer cell lines.

**Results and Discussion:** Methanolic leaf extracts showed the highest intensity of secondary metabolites and the strongest biological activity as shown in Table 1. A variety of phytochemical diversity is shown in Fig.1. A high concordance was observed between computational docking scores and experimental cytotoxicity. Specifically, Cucurbitacin E exhibited a maximum binding affinity of 10.1 kcal/mol, correlating with the potent antiproliferative effects observed in vitro. The antioxidant power of these extracts likely contributes to their chemopreventive potential by maintaining redox homeostasis. These results extend prior literature by linking specific molecular entities to observed pharmacological actions.

**Keywords:** Momordica charantia, Phytochemicals, Molecular Docking, Cytotoxicity, Breast Cancer, MCF-7, Cucurbitacin E.

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**Table 1. Yield of crude extracts from different solvents of *Momordica charantia***

| Plant Part | Solvent | Weight of Powder (g) | Extract Yield (g) | % Yield (w/w) |
|---|---|---|---|---|
| Fruit | Methanol | 100 | 9.6 | 9.6 |
| Fruit | Ethanol | 100 | 8.2 | 8.2 |
| Leaf | Methanol | 100 | 12.5 | 12.5 |
| Leaf | Hexane | 100 | 3.1 | 3.1 |
| Seed | Methanol | 100 | 10.7 | 10.7 |

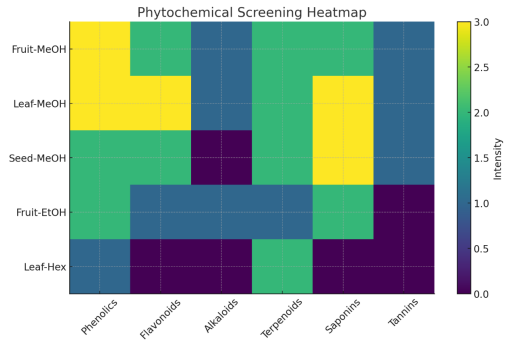


**Fig. 1 Phytochemical Screening Heatmap:** Total Phenolic Content (TPC) and Total Flavonoid Content (TFC) of various plant extracts, measured in milligrams of Gallic Acid Equivalents per gram (mg GAE/g) and Quercetin Equivalents per gram (mg QE/g), respectively. Among the samples, the Leaf-Methanol extract contains the highest concentrations of both compounds, with 75.9 mg GAE/g of phenolics and 48.7 mg QE/g of flavonoids. In contrast, the Leaf-Hexane extract shows the lowest levels, recording significantly lower values of 19.4 mg GAE/g and 12.1 mg QE/g. Overall, the data indicates that methanol is a more effective solvent for extracting these phytochemicals compared to ethanol or hexane across the fruit, leaf, and seed samples.

**Table 2: Total Phenolic content**

| Extract | Total Phenolics (mg GAE/g) | Total Flavonoids (mg QE/g) |
|---|---|---|
| Fruit-Methanol | 68.5 ± 1.2 | 41.2 ± 0.9 |
| Leaf-Methanol | 75.9 ± 1.4 | 48.7 ± 1.0 |
| Seed-Methanol | 63.1 ± 1.1 | 39.5 ± 0.8 |
| Fruit-Ethanol | 55.3 ± 0.9 | 30.6 ± 0.7 |
| Leaf-Hexane | 19.4 ± 0.5 | 12.1 ± 0.4 |

**DPPH radical scavenging activity:** The antioxidant potential is evaluated through the percentage of inhibition at two concentrations 50 µg/mL and 100 µg/mL and the calculated $IC_{50}$ value, which represents the concentration required to inhibit 50% of the free radicals. Among the tested samples, the Leaf-Methanol extract demonstrated the strongest antioxidant activity with the highest inhibition rates (81.4% at 100 µg/mL) and the lowest $IC_{50}$ value of 35.8 µg/mL. Conversely, the Leaf-Hexane extract exhibited the weakest performance, showing only 40.7% inhibition at the higher concentration and a significantly higher $IC_{50}$ of 98.4 µg/mL. While all extracts showed a dose-dependent increase in activity, the Standard (Quercetin) remained the most potent overall, achieving an $IC_{50}$ of 18.6 µg/mL.

**Table 4: DPPH radical scavenging activity**

| Extract | % Inhibition at 50 µg/mL | % Inhibition at 100 µg/mL | $IC_{50}$ (µg/mL) |
|---|---|---|---|
| Fruit-Methanol | 61.4 | 75.2 | 42.5 |
| Leaf-Methanol | 68.9 | 81.4 | 35.8 |
| Seed-Methanol | 58.7 | 73.9 | 45.2 |

| | | | |
|---|---|---|---|
| Fruit-Ethanol | 55.1 | 70.3 | 50.6 |
| Leaf-Hexane | 24.6 | 40.7 | 98.4 |
| Standard (Quercetin) | 90.4 | 96.7 | 18.6 |

**Table 5. In vitro anticancer MTT assay (MCF-7 breast cancer line)**

| Sample | Conc. (µg/mL) | % Cell Viability | $IC_{50}$ (µg/mL) |
|---|---|---|---|
| Fruit-Methanol | 50 | 55.7 | 41.3 |
| Leaf-Methanol | 50 | 48.5 | 38.9 |
| Seed-Methanol | 50 | 62.3 | 53.2 |
| Fruit-Ethanol | 50 | 66.1 | 58.4 |
| Leaf-Hexane | 50 | 81.3 | 92.7 |
| Standard (Doxorubicin) | 10 | 23.4 | 6.8 |

*in vitro* anticancer MTT assay was conducted on the MCF-7 breast cancer cell line, evaluating the cytotoxicity of various plant extracts. The data measures the percentage of cell viability at a concentration of 50 µg/mL and provides the calculated $IC_{50}$ values, which represent the concentration required to inhibit 50% of cell growth. Among the plant samples, the Leaf-Methanol extract demonstrated the highest antiproliferative activity, recording the lowest cell viability (48.5%) and the most potent $IC_{50}$ value of 38.9 µg/mL. Conversely, the Leaf-Hexane extract was the least effective, with 81.3% of cells remaining viable and a significantly higher $IC_{50}$ of 92.7 µg/mL. While the methanol-based extracts generally outperformed the ethanol and hexane counterparts, the Standard (Doxorubicin) showed the most profound inhibitory effect, achieving a much lower $IC_{50}$ of 6.8 µg/mL.

**Molecular Docking:** The molecular docking scores, measured as binding affinity in kcal/mol, for several bioactive compounds against specific target proteins associated with cancer and inflammation. Among the naturally occurring compounds listed, Cucurbitacin E exhibits the strongest binding affinity with a score of −10.1 kcal/mol against the PI3K protein. Other significant interactions include Momordicoside G with Bcl-2 (−9.2 kcal/mol) and Charantin with EGFR (−8.6 kcal/mol), while Rutin shows the lowest relative binding affinity at −7.4 kcal/mol against COX-2. Although these plant-derived compounds show high affinity for their respective targets, the Standard (Paclitaxel) maintains the most potent interaction overall, achieving a binding affinity of −11.4 kcal/mol against the PI3K protein.

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11.