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Comparative Evaluation of Antioxidant and Antitumour Activities of Curcuma-longa and Curcuma-aromatica: An Integrated Experimental and Computational Approach

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Abstract

Cancer is a major global health challenge, necessitating the discovery of effective and affordable therapeutic agents. Plant-derived natural products remain a key focus, with Curcuma longa (turmeric) and Curcuma aromatica (wild turmeric) recognised for their curcuminoid-rich phytochemistry. In this study, we comparatively evaluated the antioxidant and antitumour activities of C. longa and C. aromatica through experimental and computational approaches. Extracts were prepared using Soxhlet extraction, purified by column chromatography, and characterised by thin-layer chromatography (TLC), infrared (IR), and ultraviolet (UV) spectroscopy. Antioxidant activity was assessed by Ferric Reduction Antioxidant Power (FRAP) assay, where C. aromatica demonstrated a lower IC_{50} value compared to C. longa, indicating stronger antioxidant potential. In vitro cytotoxicity, evaluated against Dalton's lymphoma ascites (DLA) cells, revealed significant cytotoxicity for both extracts, with C. aromatica showing superior activity. Complementary molecular docking studies were performed to predict the binding affinity of major curcuminoids with cancer-related protein targets. The computational results supported experimental findings that the C. longa and C. aromatica exhibited higher binding affinity and ligand efficiency with the cancer target proteins. These results confirm the strong relationship between antioxidant and antitumour properties and highlight the therapeutic potential of C. aromatica. However, its limited availability and higher cost compared to C. longa may hinder large-scale application. Overall, this integrated study demonstrates that C. aromatica is a more efficient natural antitumour candidate, warranting further preclinical and pharmacological investigations.

Keywords: *Curcuma longa; Curcuma aromatic; antioxidant activity; cytotoxicity; molecular docking; natural anticancer agents*

1. Introduction

Cancer remains one of the most challenging global health concerns, contributing to significant morbidity and mortality worldwide [1]. Current treatment strategies, including chemotherapy, radiation, and immunotherapy, often face limitations such as toxicity, resistance, and high costs [2]. Consequently, natural products have gained renewed interest as complementary or alternative therapeutic candidates due to their bioactivity, safety, and availability [3]. The Curcuma genus, belonging to the Zingiberaceae family, is extensively studied for its pharmacological properties. Curcuma longa (turmeric) is traditionally used in Indian medicine and is well known for its curcuminoid content, primarily curcumin, demethoxycurcumin, and bisdemethoxycurcumin [4]. Curcuma aromatica (wild turmeric), though less

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commonly available, is reported to possess stronger medicinal properties and a distinct phytochemical profile [5]. The present study investigates and compares the antioxidant and antitumour activities of extracts from C. longa and C. aromatica using both in vitro assays and in silico molecular docking. The aim is to identify the more potent candidate for future anticancer drug development.

2. Materials and Methods

2.1. Plant Material and Extraction

Rhizomes of C. longa and C. aromatica were collected from authenticated sources. Samples were dried, powdered, and subjected to Soxhlet extraction using ethanol. Extracts were concentrated under reduced pressure.

2.2. Purification and Characterization

Purification and characterization of the extract were carried out using column chromatography, where fractions enriched in curcuminoids were collected. The presence of curcumin and related compounds was confirmed by thin layer chromatography (TLC) using standard references. Further analysis was performed through spectroscopy, with UV–Vis absorption recorded in the range of 200–600 nm and IR spectra obtained to identify the characteristic functional groups.

2.3. Antioxidant Assay (FRAP Method)

The antioxidant activity was determined by Ferric Reducing Antioxidant Power (FRAP) assay. IC_{50} values were calculated for both extracts.

2.4. Cytotoxicity Assay

In vitro cytotoxicity was tested against Dalton's lymphoma ascites (DLA) cells using the trypan blue exclusion method. Cell viability was recorded at different extract concentrations.

2.5. Molecular Docking

Curcumin-the major curcuminoid, was docked against cancer-related protein targets such as 4Y2G and 1OQA using AutoDock Vina. Binding energies, inhibition constants, and ligand efficiency values were calculated.

3. Results

3.1. Spectroscopic Characterization

UV–Vis spectra showed λmax at ~420-480 nm for both extracts, consistent with curcuminoid absorption.

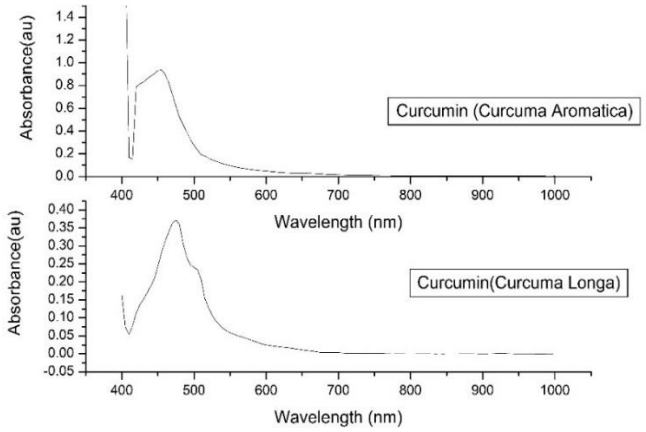

Figure 1 UV–Visible Spectra of Ethanolic Extracts of C. Longa and C. Aromatica

The FTIR spectral data of curcumin in Curcumin longa and Curcumin aromatica show characteristic peaks corresponding to their functional groups. Both samples exhibit an O–H stretch in the broad region of 3500–3200 cm^{-1}. The $–CH_3$ bending vibrations appear at 1375 cm^{-1} in both, confirming the presence of methyl groups. Aromatic C–C stretching is observed at 1601.72 cm^{-1} and at 1513.62 cm^{-1} . The C=C stretching vibrations are seen at 1626.47 cm^{-1} and 1591.65 cm^{-1}. Finally, C–O stretching appears at 1316.25 cm^{-1} and 1264.18 cm^{-1}, reflecting the linkages. In short, the data confirm the presence of common curcuminoid functional groups in both, with slight spectral shifts indicating structural variations. Figure 1 shows UV–Visible Spectra of Ethanolic Extracts of C. Longa and C. Aromatica Figure 2 shows IR Spectra Comparison of Extracts

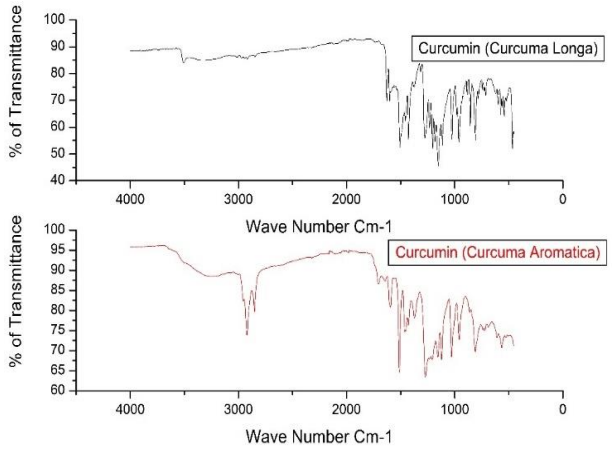

Figure 2 IR Spectra Comparison of Extracts

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3.2. Antioxidant Activity

The extract of Curcuma longa demonstrates a dose-dependent antioxidant activity, with inhibition increasing steadily up to approximately 70% at 50 µg/mL. Beyond this concentration, the activity plateaus, indicating no significant rise with higher doses. The high correlation value (R^2 = 0.9089) highlights a strong concentration–response relationship, particularly at lower concentrations. In contrast, the extract of Curcuma aromatica exhibits a rapid antioxidant response at low concentrations, reaching around 75% inhibition by just 20 µg/mL. The activity then stabilizes, maintaining levels of 85–90% at moderate concentrations. Although the correlation (R^2 = 0.8254) is slightly lower than that of C. longa, the extract demonstrates a strong radical scavenging capacity even at minimal doses. Overall, both Curcuma longa and Curcuma aromatica show significant antioxidant properties, but their response patterns differ. While C. longa provides a gradual, dose-dependent increase in activity, C. aromatica achieves higher inhibition more rapidly at lower concentrations. This suggests that C. aromatica may be more potent at small doses, whereas C. longa offers a steadier, concentration-dependent antioxidant effect. Purification and characterization of the extract were carried out using column chromatography, where fractions enriched in curcuminoids were collected. The presence of curcumin and related compounds was confirmed by thin layer chromatography (TLC) using standard references. Further analysis was performed through spectroscopy, with UV–Vis absorption recorded in the range of 200–600 nm and IR spectra obtained to identify the characteristic functional groups. Table 1 shows FRAP Assay Results (IC_{50} Values)

Table 1 FRAP Assay Results (IC_{50} Values)

Sample	IC_{50} (µg/mL)	Antioxidant activity ranking
C. longa extract	58.2 ± 2.1	Moderate
C.aromatica extract	43.6 ± 1.7	Strong

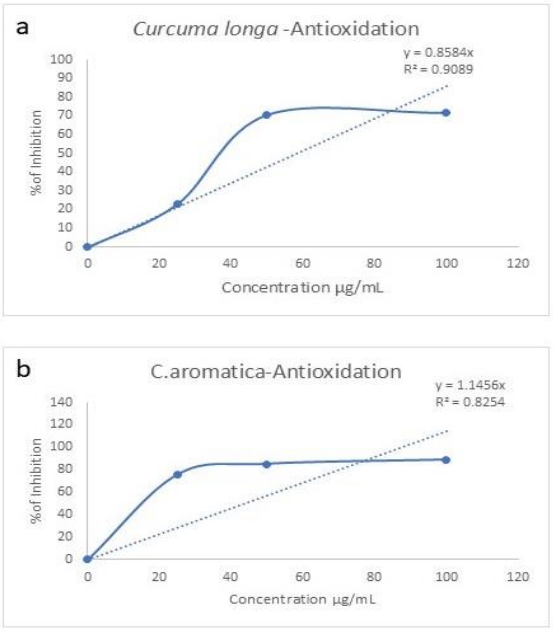

Figure 3 FRAP Assay Results (IC_{50} Values)

3.3. Cytotoxicity Assay

According to the data, C. aromatica exhibits a stronger and more rapid cytotoxic effect compared to C. longa. At the lowest tested concentration (10 µg/mL), C. aromatica causes about 62% cell death, whereas C. longa induces roughly 35–40% cell death. As the concentration increases, the cytotoxicity of both extracts rises in a dose-dependent manner. At 50 µg/mL, C. aromatica reaches ~90% cell death, while C. longa achieves ~75%. Beyond 100 µg/mL, both extracts approach maximum cytotoxicity, reaching almost 100% cell death at 200 µg/mL. The overall trend indicates that *C. aromatica* is more potent at lower concentrations, rapidly inducing cell death in DLA cells. In contrast, *C. longa* exhibits a slightly slower response, with a steady increase in cytotoxicity as the concentration rises. This suggests that while both extracts are effective against DLA cells, *C. aromatica* has a stronger anticancer potential in vitro at lower doses, whereas *C. longa* demonstrates a more gradual, concentration-dependent cytotoxic effect. Therefore, while both extracts are effective, *C. aromatica* may be preferable for rapid, low-dose applications, whereas *C. longa* provides a more controlled, concentration-dependent cytotoxic and antioxidant effect.

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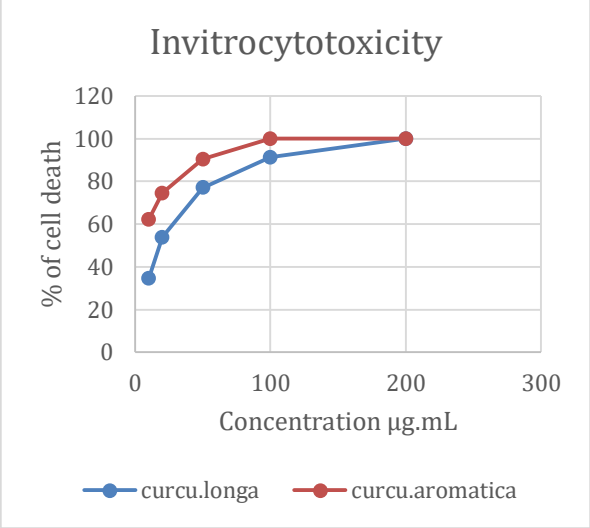

Figure 4 Cytotoxic Effect of Extracts on DLA Cells

3.4. Molecular Docking Results

The docking results indicate that curcumin exhibits a stronger binding affinity towards 1OQA compared to 4Y2G, as reflected by its more favorable binding energy (–6.99 vs. –6.11 kcal/mol), higher ligand efficiency (–0.26 vs. –0.23), and significantly lower inhibition constant (7.54 nM vs. 33.1 nM). The more negative intermolecular energy for the 1OQA complex (–10.57 kcal/mol vs. –9.69 kcal/mol) further supports the presence of stronger stabilizing interactions, including hydrogen bonding and van der Waals forces. These results collectively highlight that curcumin binds more efficiently and inhibits 1OQA more effectively than 4Y2G, suggesting that its strong interaction with cancer-related targets underpins its promising anticancer potential.

Table 2 Docking Scores of Curcumin With (a) 1OQA and (b) 4Y2G Active Sites

Active Target	Active Site and Run	BE (kcal/mol)	Ligand efficiency	inhibition constant (nM)
1OQA	2	-6.99	-0.26	7.54
4Y2G	9	-6.11	-0.23	33.1

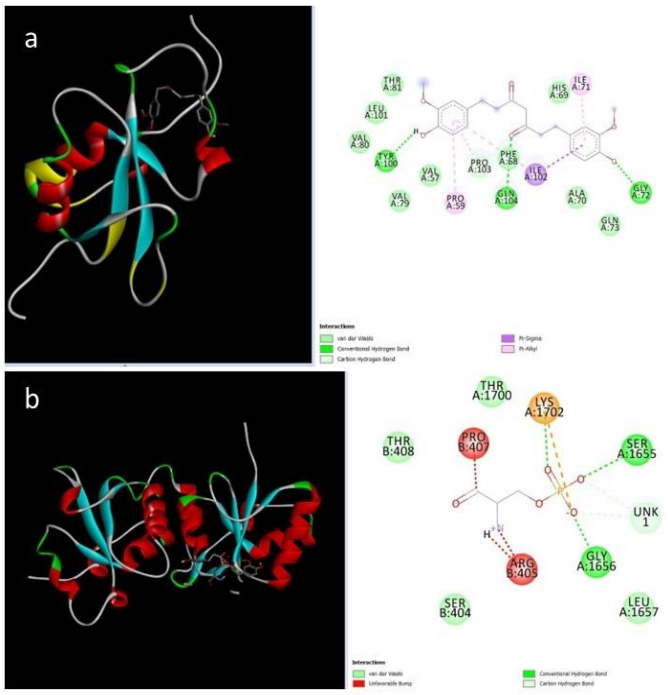

Figure 5 Docked Pose of Curcumin with (a) 1OQA and (b) 4Y2G Active Sites

4. Discussion

The findings of this study demonstrate that C. aromatica exhibits significantly stronger antioxidant and cytotoxic activities than C. longa. This may be attributed to differences in phytochemical composition and higher curcuminoid concentrations in C. aromatica [6]. Docking studies further validated the experimental outcomes. Curcumin from both C.Longa and C. aromatica shows stronger binding affinity and ligand efficiency against cancer-associated proteins. This correlation highlights the link between antioxidant defence mechanisms and cancer cell apoptosis [7]. However, practical limitations exist. While C. aromatica shows higher pharmacological potential, its limited availability, higher cost, and cultivation challenges may restrict industrial applications [8]. Strategies such as semi-synthetic analogues, nanocarrier formulations, or metabolic engineering may overcome these barriers. Figure 3 shows FRAP Assay Results (IC_{50} Values), Figure 4 shows Cytotoxic Effect of Extracts on DLA

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Cells, Figure 5 shows Docked Pose of Curcumin with (a) 1OQA and (b) 4Y2G Active Sites

Conclusion

This integrated experimental and computational study establishes that C. aromatica possesses superior antioxidant and antitumour activities compared to C. longa. The lower IC_{50} values, stronger cytotoxicity against DLA cells, and favourable docking scores highlight its therapeutic potential. Nevertheless, challenges related to availability and cost must be addressed before large-scale application. Future research should include in vivo preclinical validation, pharmacokinetics, and safety profiling.

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