INTEGRATIVE ANALYSIS OF *MORINGA OLEIFERA* PHYTOCHEMICAL COMPOSITION: INSIGHTS FROM LCMS/MS, HPTLC, HPLC PROFILING AND MOLECULAR DOCKING STUDIES

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ABSTRACT

This research presents a comprehensive investigation into the phytochemical composition of *Moringa oleifera* utilizing LCMS/MS, HPTLC, HPLC profiling and molecular docking studies. LCMS/MS analysis identified 10 key phytocompounds, including β-carbolines, octadecadiynoic acid and quercetin. HPLC technique quantified the presence of quercetin and kaempferol, gallic acid and caffeic acid. Molecular docking studies, conducted using CBDock2, unveiled potential interactions between these compounds and specific target proteins, such as β-glucosidase (PDB ID: 2ZOX). The docking results indicated favourable binding affinities for quercetin-3-*O*-glucoside, quercetin and kaempferol, highlighting their potential bioactivity.