IN SILICO MOLECULAR STUDIES OF HPLC BIOACTIVE COMPOUNDS FROM *Massularia acuminata* AS NOVEL INHIBITOR OF PHOSPHODIESTERASE-5 IN THE MANAGEMENT OF PENILE ERECTILE DYSFUNCTION

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ABSTRACT

Erectile dysfunction (ED), often colloquially referred to as impotence, is a prevalent medical condition characterized by the consistent inability to achieve or maintain an erection sufficient for satisfactory sexual performance. While occasional difficulty with erections is normal, persistent challenges in achieving or sustaining an erection can be indicative of an underlying health issue. The enzyme phosphodiesterase-5 (PDE5) is responsible for cGMP degradation; inhibiting PDE5 sustains cGMP levels, prolonging vasodilation and maintaining erections. Endothelial dysfunction, associated with reduced NO production, and factors like neurotransmitters, hormonal regulation, and inflammatory/oxidative stress contribute to the intricate biochemical landscape influencing erectile function. Understanding these pathways has led to pharmacological advancements, such as PDE5 inhibitors, providing effective interventions for ED. *Massularia acuminata*, a plant native to certain regions of Africa, has garnered attention as a potential source of therapeutic bioactive compounds due to its diverse pharmacological properties. The primary aim of this research is to conduct in-silico molecular studies on the High-Performance Liquid Chromatography (HPLC) bioactive compounds derived from *Massularia acuminata* with a focus on evaluating their potential as novel inhibitors of Phosphodiesterase-5 (PDE5) for the effective management of penile erectile dysfunction. Five lead compounds Demethoxycurcumin (-8.586), Hexadiene (-8.129), Curcumin (-7.264), Beta-Tumerone (-7.047), and Alpha Tumerone (-7.028) were shown to have better binding affinity to PDE5 than Testosterone (-6.076). ADMET studies also showed that the lead compounds have good drug-like properties that make them potential therapeutic

inhibitors of PDE5. These findings warrant further experimental investigations and emphasize the potential of these compounds in drug development efforts for penile erectile dysfunction.
Keywords: Erectile dysfunction, *Massularia acuminata,* High-Performance Liquid Chromatography,