Anti-obesity attributes; UHPLC-QTOF-MS/MS-based metabolite profiling and molecular docking insights of Taraxacum officinale

ABSTRACT

The naturopathic treatment of obesity is a matter of keen interest to develop efficient natural pharmacological routes for disease management with low or negligible toxicity and side effects. For this purpose, optimized ultrasonicated hydroethanolic extracts of Taraxacum officinale were evaluated for antiobesity attributes. The 2,2-diphenyl-1-picrylhydrazyl method was adopted to evaluate antioxidant potential. Porcine pancreatic lipase inhibitory assay was conducted to assess the in vitro antiobesity property. Ultra-high performance chromatography equipped with a mass spectrometer was utilized to profile the secondary metabolites in the most potent extract. The 60% ethanolic extract exhibited highest extract yield (25.05 ± 0.07%), total phenolic contents (123.42 ± 0.007 mg GAE/g DE), total flavonoid contents (55.81 ± 0.004 RE/g DE), DPPH-radical-scavenging activity (IC50 = 81.05 ± 0.96 µg/mL) and pancreatic lipase inhibitory properties (IC50 = 146.49 ± 4.24 µg/mL). The targeted metabolite fingerprinting highlighted the presence of high-value secondary metabolites. Molecular-binding energies computed by docking tool revealed the possible contribution towards pancreatic lipase inhibitory properties of secondary metabolites including myricetin, isomangiferin, icariside B4, kaempferol and luteolin derivatives when compared to the standard drug orlistat. In vivo investigations revealed a positive impact on the lipid profile and obesity biomarkers of obese mice. The study presents Taraxacum officinale as a potent source of functional bioactive ingredients to impart new insights into the existing pool of knowledge of naturopathic approaches towards obesity management.

Keyword: Taraxacum officinale; Antioxidant; Obesity; Metabolite profiling; Molecular docking; Lipid metabolism; Obese mice