

## Therapeutic potentials of characterized isolate from column chromatography by GC-MS and molecular docking of principle active of *Prunus domestica* L.

Kishan<sup>\*a</sup>, Rishi Kumar Shukla<sup>\*a</sup>, Abha Shukla<sup>b</sup> & Pankaj Budhlakoti<sup>c</sup>

<sup>a</sup>Department of Chemistry, Gurukula Kangri (Deemed to be University), Haridwar 249 404, Uttarakhand, India

<sup>b</sup>Department of Chemistry, Kanya Gurukula Campus, Gurukula Kangri (Deemed to be University), Haridwar 249 404, Uttarakhand, India

<sup>c</sup>Central Laboratory, Patanjali Food and Herbal Park Pvt. Ltd., Padartha, Haridwar 249 404, Uttarakhand, India

E-mail: prajapati75kishan@gmail.com, rkshukla@gkv.ac.in

Received 27 December 2023; accepted (revised) 28 June 2024

Chromatographic techniques aid in isolating and separating phytoconstituents from natural products, enabling the discovery of innovative compounds of pharmacological and physiological importance. The present study is focused on isolation and identification of the compounds in column chromatography-derived fraction using GC-MS and its biological activities. The ethyl acetate extract of the leaves of *Prunus domestica* L. has been column chromatographed using gradient of ethyl acetate in petroleum ether as solvent. This has yielded a red coloured fraction/band (RCF) (approximately 130 mg), which has further been analysed by GC-MS for the identification of bioactive phytoconstituents. The RCF has been analysed for antioxidant activity by DPPH method which has shown an IC<sub>50</sub> value of 43.895 mg/mL. The antibacterial activity of RCF has been assessed by agar well diffusion method against *E. coli* which has shown the zone of inhibition of 17 mm. Stigmast-5-en-3-ol, oleate (31.77%) is identified as the major phytoconstituent and molecular docking of this major constituent has been carried out to observe its interactions with heme oxygenase and DNA gyrase protein chains.

**Keywords:** *Prunus domestica* L., Column chromatography, GC-MS, Antioxidant activity, Antibacterial activity, Molecular docking