

**Title:** In vitro anti-leishmanial activity of *Prunusn armeniaca* fractions on *Leishmania tropica* and molecular docking studies

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**Abstract**

Cutaneous leishmanaisis (CL) is a neglected tropical disease that currently affects people among 102 countries and causes significant mortility and morbidity. Current chemotherapeutic interventions is unsatisfactory and has various limitations that highlight the necessity to develop effective and safe therapeutic approaches from natural products. *Prunus armeniaca* (L.) is a member of the Rosaceae, subfamily Prunoideae, shows anticancer, antitubercular, antimutagenic, antimicrobial, antioxidant, and cardioprotective activities. Here we fractionated the leaves extract of this highly medicinally important plant for antileishmanial activity. In the current study, the leaves extract was fractionated and characterized using column and thin layer chromatography by n-hexane, ethyl acetate, and methanol solvents. Twelve fractions were isolated and subjected for evaluation of their cytotoxicity and in vitro antileishmanial activity against promastigotes and amastigotes of *Leishmania tropica*. Among all fractions used, the fraction (F7) exhibited the strongest antileishmanial activity. The bioactive fraction was further characterized by spectroscopy (FTIR, UV–Vis), and GC-MS analysis. The in silico docking was carried out to find the active site of PTR1. All derived fractions exhibited toxicity in the safety range $IC_{50}$ > 100 μg/ml. The fraction (F7) showed significantly the highest antipromastigotes activity with $IC_{50}$11.48 ± 0.82 μg/ml and antiamastigotes activity with $IC_{50}$ 21.03 ± 0.98 μg/ml compared with control i.e. 11.60 ± 0.70 and 22.03 ± 1.02 μg/ml respectively. The UV–Vis spectroscopic analysis revealed the presence of six absorption peaks and the FTIR spectrum revealed the presence of alkane, aldehyde, carboxylic acid, thiols, alkynes, and carbonyls compounds The GC–MS chromatogram exhibited the presence of nine compounds: (a) benzeneethanol, alpha, beta dimethyl, (b)carbazic acid, 3-(1 propylbutylidene)-, ethyl ester, (c)1, 2-benzenedicarboxylic acid, diisooctyl ester, (d)benzeneethanamine a-methyl, (e)2aminononadecane, (f)2-heptanamine-5-methyl, (g)cyclobutanol, (h)cyclopropyl carbine, and (i)nitric acid, nonyl ester. Among all compounds, the 1, 2-benzenedicarboxylic acid, diisooctyl ester

bound well to the PTR1 receptor. Fraction (F7) showed acceptable results with no cytotoxicity. However, in vivo studies are required in the future.

**Biography**

Dr. Naveeda Akhtar Qureshi working as an associate Professor in the Parasitology lab of Quaid-i-Azam University Islamabad, Pakistan. She has produced 47 M.phil and 4 Ph.D students. Currently, she is supervising 6 M.phil and 5 Ph.D students. She has published more than 51 papers in reputed journals. She attended national and international conferences.

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