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Potential drug candidates against Hepatitis C virus: *In silico* screening of phytoconstituents from *Phyllanthus fraternus* G.L. Webster

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Hepatitis C is a liver inflammatory disease caused by the Hepatitis C virus. *Phyllanthus fraternus* G.L. Webster, commonly called Gulf leaf-flower, is an important medicinal plant and possesses hepatoprotective activity against hepatitis. Here, we have determined and characterized the active ingredients from the leaf extract of *P. fraternus* by gas chromatography-mass spectrometry (GC-MS) analysis. It resulted in the identification of fifteen compounds, which are the first to be reported from *P. fraternus*. For finding the compounds responsible for HCV, identified compounds were docked against important enzymes of HCV virus metabolism viz: HCVNS3 enzyme, HCVNS5, and hepatic damage indicator enzymes AST and ALT. To ensure drug-likeness, the pharmacokinetic, physicochemical, and toxicity properties of the compounds were also evaluated. The study has demonstrated the presence of seven hepatoprotective compounds (alpha-cadinol, elemol, 1,6-germacradien-5-ol, phytol, carissanol dimethyl ether, phlytetralin and 3-furanmethanol, alpha-(3,4-dimethoxyphenyl) tetrahydro-3-hydroxy-4-veratryl- in the leaves extract of *P. fraternus* against the hepatitis C virus.

Keywords: Blood brain absorption, CaCO₂ permeability, Gulf leaf-flower, Human intestinal absorption, Liver