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Abstract

Background: Antioxidant and antihistamine agents from *Barleria noctiflora* L.f. as natural source due to the existing modern medicine give various adverse effects to overcome these problems with natural products.

Methods: *B. noctiflora* leaves extract was fractionated with column chromatography; the homogenized fractions were monitored with thin layer chromatography (TLC) and characterized by using UV–visible, FT-IR, ^{1}H NMR, ^{13}C NMR and mass spectrometry spectral studies. The volatile phytoconstituents of *B. noctiflora* extract were analysed by gas chromatography–mass spectrometry. Phytoconstituents from *B. noctiflora* leaves extract were screened for their antioxidant and antihistamine potential *in vitro* (2,2-diphenyl-1-picrylhydrazyl radical scavenging activity, 2,2′-azinobis-3-ethylbenzothiozoline-6-sulfonic acid radical decolouration assay, nitric oxide radical scavenging activity, superoxide radical scavenging activity and hydrogen peroxide radical scavenging activity) and *in silico* (molecular docking), respectively.

Results: Antioxidant and antihistamine barlerinoside has been isolated and characterized from the leaves of *B. noctiflora* L.f. Barlerinoside revealed their free-radical scavenging ability on OH^-, $OH^{\bullet}$, NO^-, O_2^- and H_2O_2 radicals and found high percentage inhibition against OH^- radical at the IC_{50} value of 50.45 ± 2.52 µg. The methanol (MeOH) extract of *B. noctiflora* leaves contains cyclotene; N,N-dimethylglycine; tetrahydrocyclopenta [1,3] dioxin-4-one; phenol, 2-methoxy-; benzofuran, 2-methyl-; 1,4:3,6-dianhydro-α-D-glucopyranose; 2-methoxy-4-vinylphenol; 1,3;2,5-dimethylene-L-rhamnitol; levoglucosan and bicyclo [2.2.2]oct-7-ene-2,3-dione as being the major compounds. Among phytoconstituents present in the extract, the hexestrol; 1,2-benzenedicarboxylic acid, bis(2-methylpropyl) ester; 1-(3,6,6-trimethyl-1,6,7,7a-tetrahydrocyclopenta[c] pyran-1-yl) ethanone; megastigmatrienone; furan interacted with histamine H_1 receptor and bind at GLU-177 and ASP-178 with high binding energy score –13.95, –13.41, –12.56, –12.03, and –11.72 kcal/mol, respectively, and the expected hydrolysed products of compound-1a and compound-1b from barlerinoside showed –8.91 and –8.68 kcal/mol binding energy against the histamine H_1 receptor. This showed that the active ligands exactly bind with active binding site of the protein.

Conclusions: We can conclude that isolated barlerinoside from *B. noctflora* L.f. has potent antioxidant activity against synthetic free radicals and antihistamine activity against histamine H_1 receptor.

Keywords: antihistamine, antioxidant, *Barleria noctiflora*, free-radical scavenging, gas chromatograph and mass spectrum, histamine H_1 receptor

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Introduction

Barleria noctiflora L.f. is a tropical weed belonging to Acanthaceae family habituated throughout the tropical region of India and is commonly known as Udamully in Tamil and Bajardanti in Rajasthan. It is a shrub up to 0.5–1.0 m height, leaves are oblong, hairy stem and has white flower [1]. Amongst *Barleria* species, *Barleria prionitis*, *Barleria greenii* and *Barleria albostellata* contain antifungal activity, acetylcholinesterase inhibitory activity, antioxidant activity [2], mast cell stabilization and membrane protection activity [3]; *Barleria argillicola* contains antibacterial activity [4] and anticancer activity [5]; *Barleria bispinosa* contains antihyperglycemic and antihyperlipidemic effects [6] and *Barleria lupulina* contains antiarthritic activity, immunomodulatory activity [7] and anti-diabetic activity [8]. Our earlier report