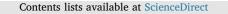
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Anti-inflammatory and antioxidant potential of Guaianolide isolated from *Cyathocline purpurea*: Role of COX-2 inhibition



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ABSTRACT

Background: Inflammation activated by oxidative stress can cause various diseases, such as asthma, rheumatoid arthritis, cancer, diabetes, etc. Plant constituents with sesquiterpene lactones possess antioxidant and anti-inflammatory properties.

Aim: To determine the antioxidant and anti-inflammatory potential of isolated phytoconstituent from *Cyathocline purpurea* Buch-Ham ex D (CP). Don in laboratory animals. Furthermore, to understand the interactions involved in the binding of this compound to cyclooxygenase-2 (COX-2) via computational docking.

Methods: Phytoconstituent was isolated, purified and well characterized (using IR, NMR, and MS) from ethyl acetate fraction of CP methanolic extract. It was then evaluated for its in-vitro antioxidant activity against 1,1-diphenyl-2-picrylhydrazyl (DPPH), hydrogen peroxide (H_2O_2) and hydroxyl (OH) radical assays as well as in-vivo anti-inflammatory potential against carrageenan-induced paw edema model in rats. The molecular docking study was performed against the crystal structure of COX-2 to evaluate the binding potential of phytoconstituent towards this enzyme.

Results: The isolated compound 6 α -hydroxy-4 [14], 10 [15]-guainadien-8 α , 12-olide (HGN) showed significant (p < 0.001) antioxidant activity with IC₅₀ values of 76 µg/mL. Administration of HGN (10 and 20 mg/kg) significantly (p < 0.001) reduced the increased paw volume after subplantar administration of carrageenan. It also exhibits good binding affinity towards with COX-2 with a docking score of - 8.98 and Glide binding energy of - 36.488 kcal/mol shedding light on the potential mechanism of anti-inflammatory action.

Conclusions: The presence of hydroxyl group in HGN provides a credential to its in-vivo anti-inflammatory and in-vitro antioxidant activities. Furthermore, the good binding affinity of HGN for the active site of COX-2 may open novel vistas in therapeutic option with natural antioxidants like *Cyathocline purpurea* to treat various inflammatory disorders.

1. Introduction

Inflammation is an imperative physiological reaction which occurs in retort to various detrimental agents (e.g. bacterial infection, physical trauma, chemicals or any other phenomenon) ultimately aiming to execute limiting damage and promoting tissue repair [1]. Inflammatory processes are associated with many degenerative diseases such as rheumatoid arthritis, shoulder tendinitis, gouty arthritis, polymyalgia rheumatica, heart disease, asthma, and inflammatory bowel [2]. Inflammation triggered by oxidative stress can affect various system leading to neurodegenerative disorders including Alzheimer's, cardiovascular diseases, arthritis, diabetes, epilepsy, chronic fatigue syndrome, hepatotoxicity, neurotoxicity, nephrotoxicity, etc. [3–11].

Now a day non-steroidal anti-inflammatory drugs are adopted for the alleviation of inflammation and pain. However, there is a restriction on the utility of such drugs due to their side effects like gastric ulcer,

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List of abbreviations: CMC, carboxymethyl cellulose; COX-2, cyclooxygenase-2; CP, Cyathocline purpurea Buch-Ham ex D.; DPPH, 1, 1-diphenyl-2-picrylhydrazyl; Glide, Grid-based Ligand Docking with Energetics; HGN, 6α-hydroxy-4[14], 10[15]-guainadien-8α, 12-olide; RMSD, Root Mean Square Deviation; ROS, reactive oxygen species

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