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# GC-MS analysis of the alkaloid extract of *Epdedra equisetina* and *in silico* anti-inflammatory activity of its alkaloids

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*Epdedra equisetina* is a potential medicinal plant in Tajikistan. It has been used for a long time in Tajik folk medicine for colds, joint pain, rheumatism, malaria, stomach and liver disorders. The alkaloid extract of *Epdedra equisetina* is obtained by acid-base extraction and analyzed by gas chromatography-mass spectrometry (GC-MS) and column chromatography (CC). The alkaloid extraction yield of *Ephedra equisetina* is 1.57%. Four alkaloids, namely ephedrine (pseudoephedrine), 2,3,4-trimethyl-5-phenyloxazolidine, *trans*-1,2-dimethyl-3-phenylaziridine and 3,4-dimethyl-2,5-dipheryloxazolidine have been identified in the alkaloid extract of *Epdedra equisetina*. *In silico* anti-inflammatory activity of *Epdedra equisetina* alkaloids have been tested against inhibition of cyclooxygenases-1 enzyme (COX-1) (PDB code 3N8Z), cyclooxygenases-2 enzyme (COX-2) (PDB code 3LN1), and P38 mitogen-activated protein kinase (p38MAPK) (PDB code 1OZ1). Celecoxib has been used as a positive control. Molecular docking values of alkaloids in *Epdedra equisetina* range between –5.2 and –9.4 kcal/mol. The value for the reference drug (celecoxib) ranges between –6.6 and –12.2 kcal/mol. 3,4-Dimethyl-2,5-diphenyloxazolidine shows the highest molecular docking values of –7.0, –9.4, and –7.8 kcal/mol for COX-1, COX-2, and p38MAPK proteins, respectively. 3,4-Dimethyl-2, 5-diphenyloxazolidine can act as a natural alternative inhibitor of the COX-2 protein.

**Keywords:** *Ephedra equisetina* Bunge, Alkaloids, GC-MS analysis, Ephedrine, Anti-inflammatory activity