

STRUCTURE ACTIVITY RELATIONSHIP STUDY ON ISOLATED COMPOUNDS AND STANDARDISED EXTRACT PREPARATION FROM *Prismatomeris malayana*

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OBJECTIVE

The objective was to isolate and identify the active anti-inflammatory compound(s) from *Prismatomeris malayana* Ridley using several bioassays. The computational study will be constructed on the structure and bioactivity of the active compound and its analogues using QSAR technique. Finally, the suitability of this plant species will be evaluated for anti-inflammatory product formulation

METHOD

The methanol extracts of leaf, stem and root of *Prismatomeris malayana* were evaluated for their anti-inflammatory activities based on the hyaluronidase inhibitory and TPA induced mouse ear oedema bioassay. Further studies were carried out on the most active extract, *i.e.* the leaf extract, and were further subjected to fractionation through successive solvent-solvent partitioning to obtain petroleum ether, chloroform, ethyl acetate and water fraction. Further fractionation and purification was carried out on the chloroform fraction. For the activity assessment, each fraction was submitted to hyaluronidase inhibitory bioassay.

In order to obtain the triterpenoid saponins extract from the dried and powdered leaves of *Prismatomeris malayana*, a systematic single factor study on the effect of extraction parameters such as temperature, time, solvent volume and concentration of ethanol on the content of triterpenoids saponins was carried out.

The second approach in this study could be categorised as the preliminary drug development study. Several ursolic acid analogues (ursane skeleton) were prepared and their IC₅₀ values on the anti inflammatory activity were evaluated. The ursane skeleton

compounds, their biological data and a variety of descriptors were computed using the CODESSA software in order to come out with the regression model. The quantitative structure activity relationship studies (QSAR) used the quantum chemical method to perform conformational analysis and properties calculation. The MOPAC was used for geometrical optimisation.

RESULTS

The methanol leaf extract displayed marked anti-inflammatory effects on both assays as compared to reference compound. From the chloroform fraction of the leaf extract, a major and active component was isolated. The structure was determined as ursolic acid by means of spectral techniques.

From the optimised extraction procedure, an extract with triterpenoids saponins content of at least 10% ursolic acid equivalent was obtained. The prototype cream for skin and health care were developed using the standardised extract as the active ingredient.