



## Identification, isolation, and characterisation of bioactive compounds from *Hypoestes aristata*(Acanthaceae)

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### Abstract

The aim of this study was to identify and isolate potential biologically active compounds from the stems of *Hypoestes aristata* (Vahl) Sol. ex Roem. & Schult (Acanthaceae) and test them for their biological activities. The identification and isolation of potential bioactive compounds was achieved through chromatographic techniques such as column chromatography, preparative thin layer chromatography (PTLC), preparative high pressure liquid chromatography (Prep-HPLC), liquid chromatography-solid phase extraction-mass spectrometry (LC-SPE-MS), and ultra-high performance liquid chromatography-quadrupole time-of-flight mass spectrometry (UHPLC-qTOF-MS). The characterisation and structural elucidation of the isolated compounds was mainly facilitated by spectroscopic/spectrometric techniques including 1D NMR (1HNMR, 13C-NMR, dept-135) and 2D NMR (COSY, HSQC, HMBC, NOESY) and high-resolution mass spectrometry (HRMS).

From the stems of *Hypoestes arisata*, ten compounds that belong to the class of lignans were isolated and characterised. Among these compounds, four known butyrolactone lignans hinokinin, savinin, and cubebins; three new butyrolactone lignans (7S,8S,7'S,8'R)-7'-acetoxy-7-hydroxyhinokinin, (7S,8S,7'S,8'R)-7-acetoxy-7'-hydroxyhinokinin, and (7S,8S,7'S,8'R)-7,7'-diacetoxyhinokinin; and three new butyrolactol lignans.

(7R,8S,9R,7'R,8'R)-7,7'-diacetoxy-cubebin, 7,7'-diacetoxy-cubebin, and (7S,8R,9S,7'R,8'R)-7,7'-diacetoxy-cubebin were isolated. The absolute configurations of novel compounds were determined from their electronic circular dichroism (ECD) spectra and by derivatisation into (S) and (R)-MTPA esters. The newly isolated compounds are novel compounds. To the best of our knowledge, this is the first research which has isolated these compounds and confirms their absolute configurations from *H. aristata*.

The compounds were screened for inhibition of a HIV-1 protease enzyme, hinokinin, (7S,8S,7'S,8'R)-7'-acetoxy-7-hydroxyhinokinin, (7S,8S,7'S,8'R)-7,7'-diacetoxyhinokinin, and (7R,8S,9R,7'R,8'R)-7,7'-diacetoxy-cubebin showed moderate protease inhibition at concentrations below 60  $\mu$ M and other compounds showed insignificant inhibitory activities at concentrations above 100  $\mu$ M. Additionally, the compounds (7S,8S,7'S,8'R)-7'-acetoxy-7-hydroxyhinokinin, (7S,8S,7'S,8'R)-7,7'-diacetoxyhinokinin, and (7R,8S,9R,7'R,8'R)-7,7'-diacetoxy-cubebin were also tested for cytotoxicity against the MCF-7 and MDA-MB-231 cancer cell lines and found to be inactive at concentrations below 90  $\mu$ M.

### Biography

A well-educated Organic Chemist with a strong research & development background. Has worked in world-class, research environments; with a focus on driving innovation and forward thinking research methodologies. Implements robust project & research management frameworks; has the ability to identify inefficiencies, is able to deliver projects on-time, within budget and ensure the integrity of the data. Has a proven track record in managing multiple research studies, and is a subject matter specialist in the initiating, implementing, overseeing, and closure of research programmes. Extensive testing, analytical and data interpretation experience. A true problem solver who thrives on driving quality and compliance to the highest level. Has solid communication skills, meticulous attention to detail and creates a professional and result orientated environment.

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