Identification of phenanthrene derivatives in *Aerides rosea* (Orchidaceae) using on-line hyphenated systems

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Aim of the study

In our continued efforts to contribute to the general knowledge about chemical diversity of orchids, our investigations focused on the Aeridinae subtribe. After our previous phytochemical study of *Vanda coerulea*, which has led to the identification of stem-specific phenanthrene derivatives, a closely-related species, *Aerides rosea* Lodd. ex. Paxton, has been explored.

Methodology

A dereplication strategy was developed using an HPLC-DAD-HRMS/MS targeted method and applied to fractions from *A. rosea* stem extract. Then, the characterization of unknown minor compounds was performed by the hyphenated HPLC-DAD-MS-SPE-UV-NMR system.

Results

The analyses of two fractions (F1 and F2) by the hyphenated HPLC-DAD-MS-SPE-UV-NMR system permitted the identification of five additional minor constituents including one phenanthropyran (5), two phenanthrene (1 and 4) and two dihydrophenanthrene (2 and 3) derivatives. The full set of NMR data of each compound was obtained from microgram quantities.

![Image](image1.png)

HPLC chromatograms of the fractions of *A. rosea* stems (recorded at 260 nm). Unknown compounds are denoted 1 s. Stationary phase: Sunfire C18 150 mm x 4.6mm i.d. 3.5 µm; Flow: 1 mL/min; Injection volume: 5 µL (5mg/mL). Mobile phase: A - water + 0.1% A.F.; B - ACN+ 0.1% A.F. Linear gradient (time): 0 min: 20%, 3 min: 30%, 11 min: 35%, 25 min: 50%, 37-46 min: 100%.

![Image](image2.png)

1H NMR spectra of the compounds 1-5 identified in *A. rosea* by the hyphenated HPLC-DAD-MS-SPE-UV-NMR system (MeOD-d4 at 500 MHz).

![Image](image3.png)

HMBC experiment of aerosanthrene (1) [MeOD-d4 at 500 MHz].

Conclusion

Nine secondary metabolites were characterized in *A. rosea* stems, utilizing high resolution hyphenated analytical tools. Two of them are newly described phenanthrene derivatives: aerosanthrene (5-methoxyphenanthrene-2,3,7-triol) and aerosin (3-methoxy-9,10-dihydro-2,5,7-phenanthrenetriol).

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