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METABOLITE PROFILING OF THE AERIAL PARTS OF *Actinocephalus divaricatus* (KOERN.) SANO (ERIOCAULACEAE) BY LC-ESI-MS

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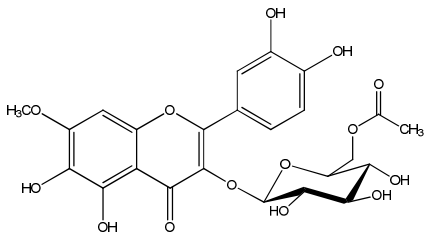
Abstract: The sect. *Actinocephalus* (Koern.) Ruhland, belonging to the genus *Paepalanthus* has recently been elevated to a new genus *Actinocephalus* (Koern.) Sano [1]. Chemical and biological studies of plant species belonging to the genus *Actinocephalus* are scarce in the literature. To our knowledge no investigation has been performed until now concerning the chemical composition and biological studies of aerial parts of *Actinocephalus divaricatus*. Thereby, we decided to carry out an analytical study by LC-ESI-MS/MS to developed to rapidly identify and define the metabolite profiling of the aerial parts of *A. divaricatus*. The metabolite profile using HPLC-ESI-MS was carried out for the methanol extract of aerial parts of *A. divaricatus*, separately. Later MS/MS the fragmentation experiments allowed identify the metabolites in the chromatographic peaks. The characterization and differentiation of the three plant parts (capitulae, scapes and leaves) was realized using metabolites libraries and databases. Since the high-resolution device with Xcalibur 2.0 software, allowed determine the mass and the molecular formulas with high degree of similarity for each peak detected. The analysis of the ESI-MS/MS of the methanolic extract revealed the presence of the flavonoids in the capitulae, scapes and leaves. The naphthopyranones were also identified only in capitulae and in the leaves. Therefore, in total were proposed the structure of 14 flavonoids and 4 naphthopyranones. Among the proposed compounds, we can mention methoxylated flavonols and acyl glycosylated as well as glycosylated derivatives of paepalantine. These chemical characters reinforce *Actinocephalus* as a distinct genus separated from *Paepalanthus* as proposed by Sano [1, 2]. In addition, the fractionation of the methanolic extract of the leaves by Sephadex LH-20/HPLC-IR yielded the new flavonoid acyl glycosylated 6-hydroxy-7-methoxyquercetin-3-*O*-(6"-*O*-acetyl)-*β*-D-glucopyranoside (Figure 1). The structures of the compounds were determined by analysis of data obtained by mono and bidimensional NMR. The isolation of these substances also helped identify other molecules that had similar fragmentation patterns. So this study allowed the full study of the capitulae, scapes and leaves of the *A. divaricatus*, and the proposal of structures of unknown compounds.

Figure 1. Structure of 6-hydroxy-7-methoxyquercetin-3-*O*-(6"-*O*-acetyl)-*β*-D-glucopyranoside.



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