

Chemical Constituents of the Methanol 90% Fraction Derived from the Total Extract of *Coccoloba cowellii* Leaves [†]

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Abstract: *Coccoloba cowellii* Britton (Polygonaceae, order Caryophyllales) is an endemic and critically endangered plant species that only grows in the municipality of Camagüey, province of Cuba. Preliminary investigation of its total methanolic extract led to the discovery of a promising antifungal activity. The major constituents of the aforementioned extract were glucuronides and glycosides of myricetin and quercetin, proanthocyanidins (tentatively characterized by means of HRMS), as well as epicatechin-3-O-gallate, catechin, epicatechin and gallic acid (tentatively characterized by using HRMS and authentic standards). A UHPLC-ESI-QTOF-MS analysis of the methanol 90% fraction (MeOH90-F) derived from the total extract, allowed the identification of flavonoid glycosides/glucuronides, lignin oligomers, and methoxyflavonoids as the main constituents of that fraction. A combination of flash chromatography, 1D and 2D NMR, and NMR-based machine learning tool “Small Molecule Accurate Recognition Technology” (SMART 2.1, available at <https://smart.ucsd.edu/classic>) allowed the isolation from MeOH90-F of quercetin and four methoxyflavonoids: 3-O-methylquercetin, myricetin 3,3',4'-trimethyl ether, 6-methoxymyricetin 3,4'-dimethyl ether and 6-methoxymyricetin 3,3',4'-trimethyl ether. This report contributes to a better understanding of the phytochemistry of the genus *Coccoloba*.

Keywords: *Coccoloba cowellii*; Polygonaceae; UHPLC-ESI-QTOF-MS; methoxyflavonoids

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1. Introduction

2. Material and Methods

3. Results and Discussion

4. Conclusions

Institutional Review Board Statement:

Informed Consent Statement:

Data Availability Statement:

References