Supplementary Information

Effect of Endophytic Fungal Associations on the Chemical Profile of *in vitro Vochysia divergens* Seedlings

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Hierarchical clustering analysis (HCA)

Chromatographic bands observed in the HPLC analysis of *in vitro V. divergens* seedlings inoculated with endophytic fungi from the dry and wet periods were used in the HCA (hierarchical clustering analysis) compared to the control sample (seedlings without fungi inoculation) and the results were expressed as dendrograms. The metric used in the analysis was the Euclidean distance as suggested by Ferreira.[1] In addition, the Ward's minimal variance method[2] was employed to perform the agglomerative hierarchical clustering procedure. Ward's minimal variance method is based on the sum of squares of deviations from the cluster centroid. Ward's method analyzes the possible pairs of joined clusters that will produce the smallest increase in the intra-cluster sum of squares.[3]

References

1. Ferreira, M. M. C. In *Quimiometria: Conceitos, Métodos e Aplicações*, 1ª ed.; Unicamp: Campinas, São Paulo, Brazil, 2015, p. 496.

2. Ward, J. H.; *J. Am. Stat. Assoc.* **1963**, *58*, 236.

3. Murtagh, F.; Legendre, P.; *J. Classif.* **2014**, *31*, 274.

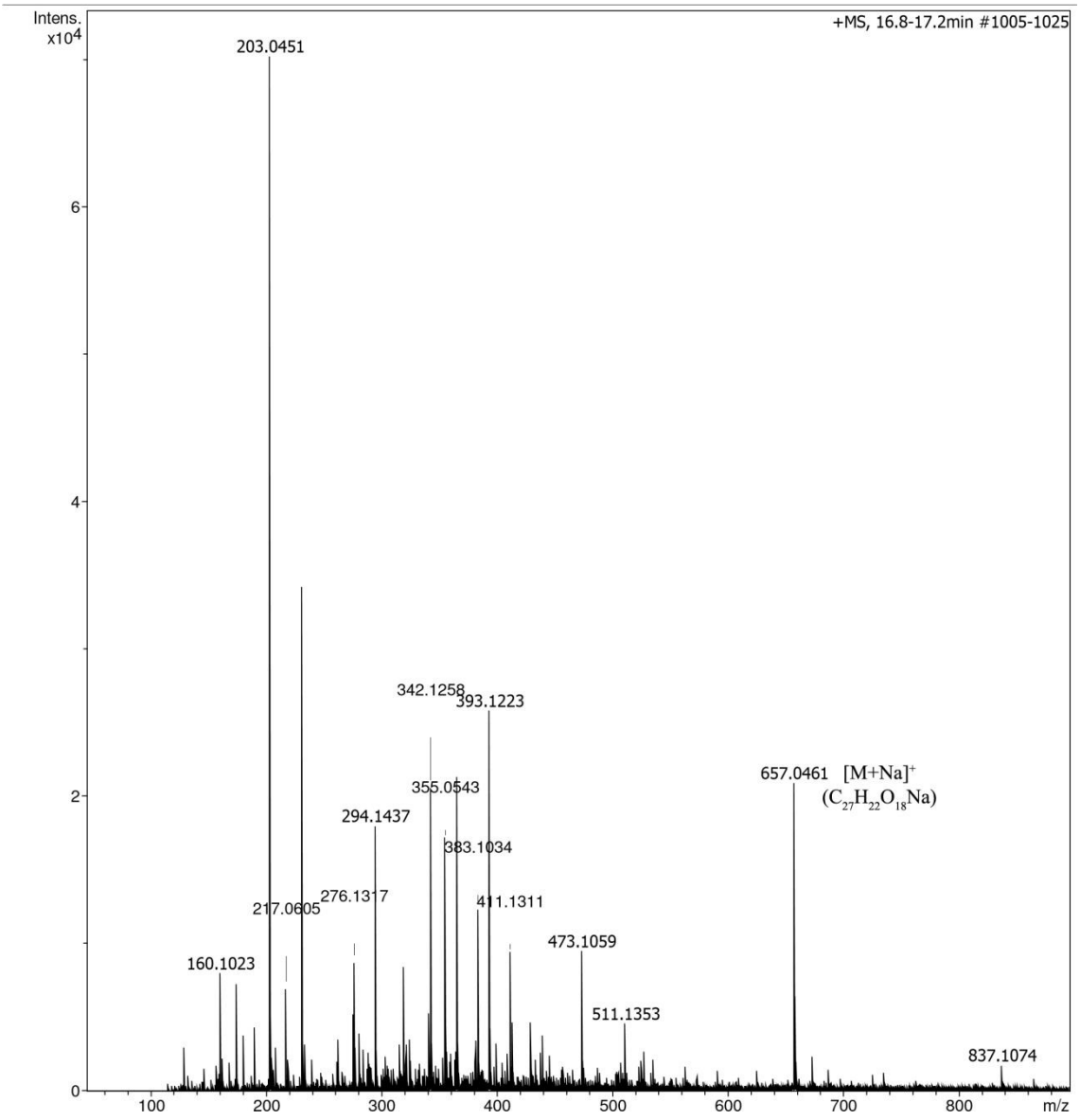

Figure S1. ESI mass spectrum obtained in the positive ion mode for compound **1**.

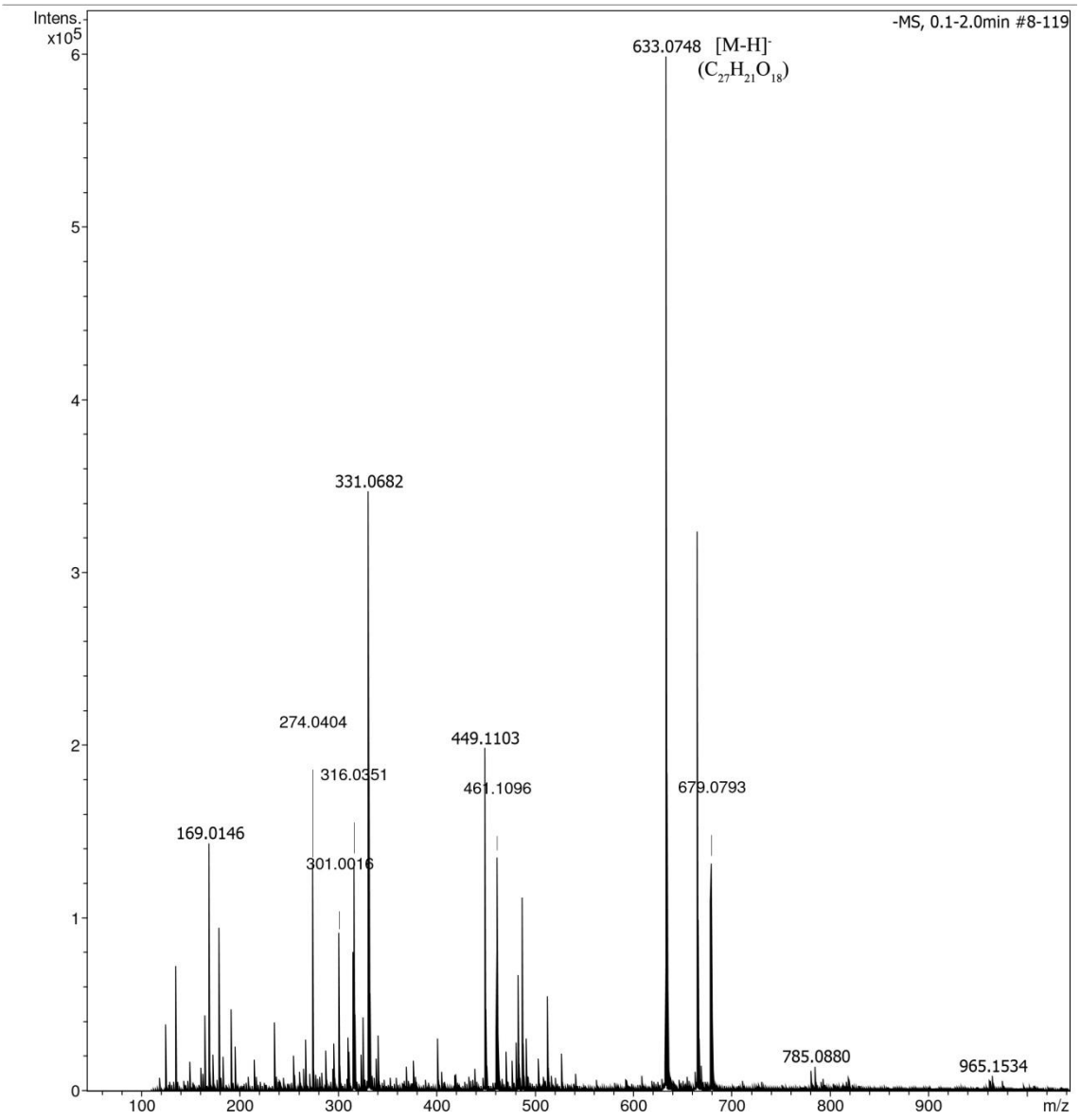

Figure S2. ESI mass spectrum obtained in the negative ion mode for compound **1**.

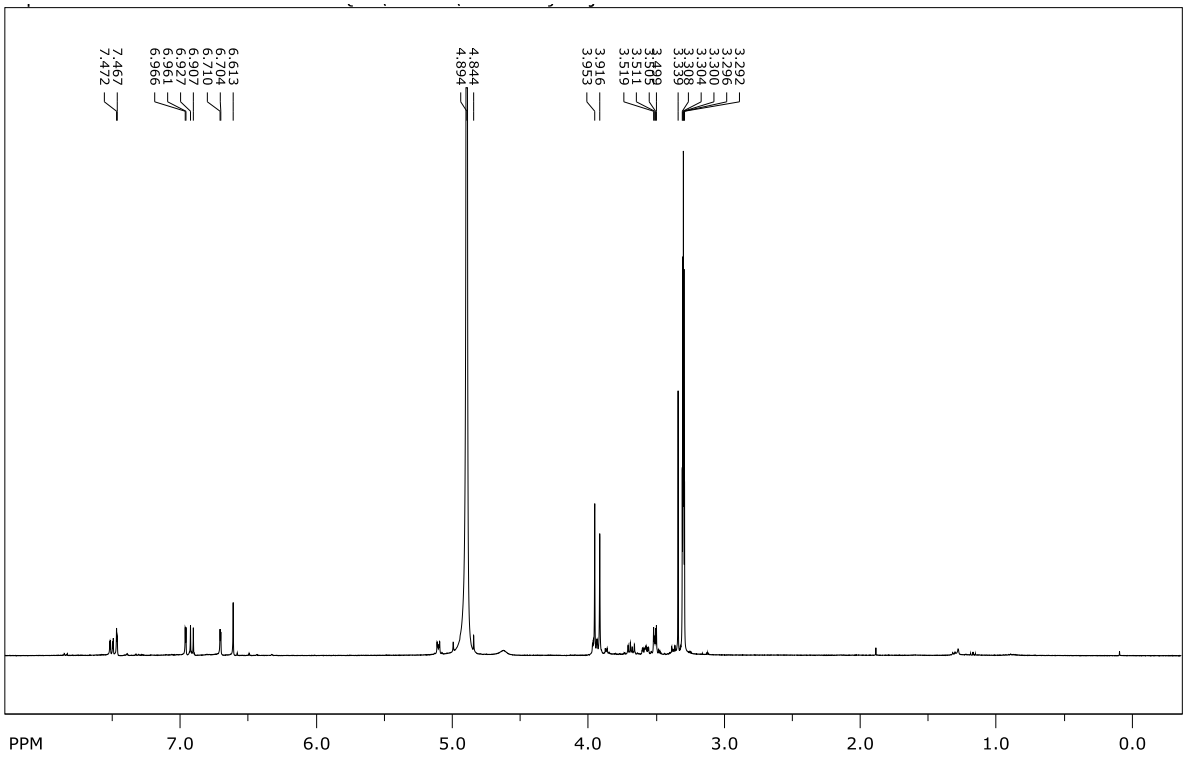

Figure S3. ^{1}H NMR spectrum (400 MHz, CD_3OD) of compound **3**.

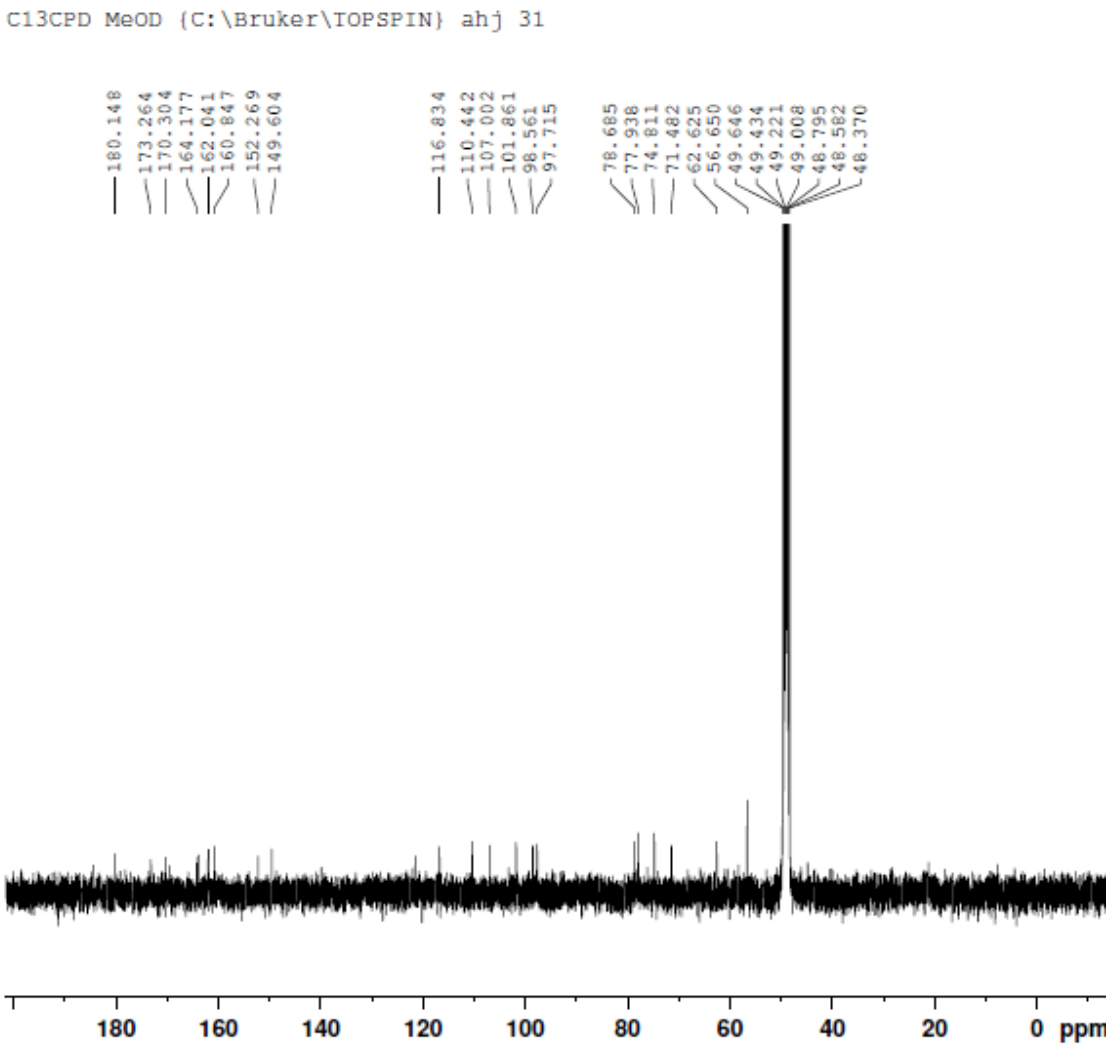

Figure S**4.** ^{13}C NMR spectrum (100 MHz, CD_3OD) of compound **3**.

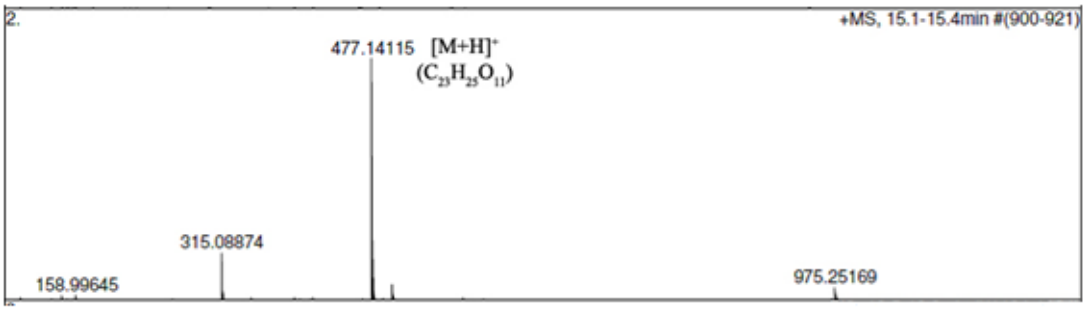

Figure S5. ESI mass spectrum obtained in the positive ion mode for compound **3**.

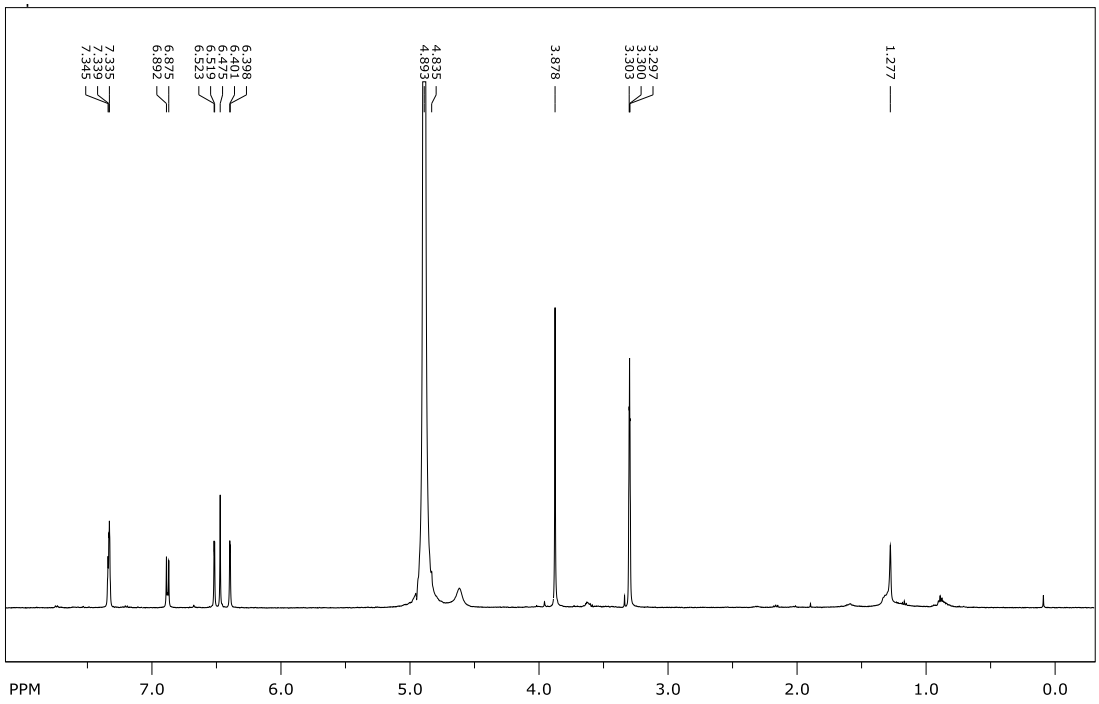

Figure S6. ^{1}H NMR spectrum (500 MHz, CD_3OD) of compound **4**.

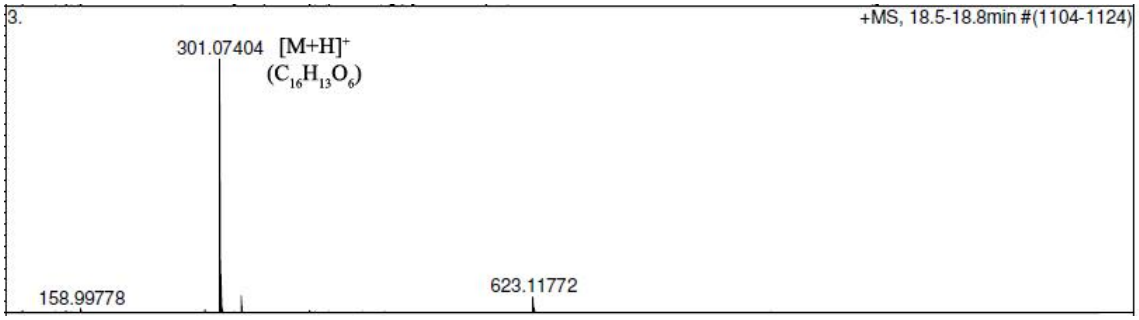

Figure S7. ESI mass spectrum obtained in the positive ion mode for compound **4**.

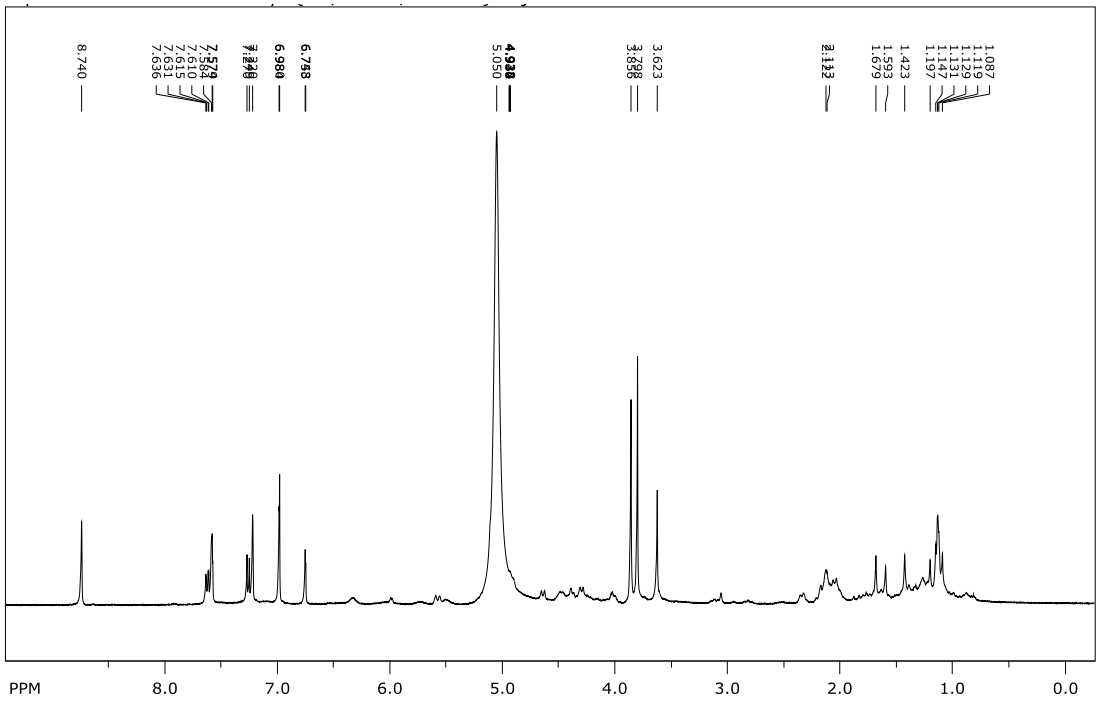

Figure S8. ^{1}H NMR spectrum (400 MHz, C_5D_5N) of compound **5**.

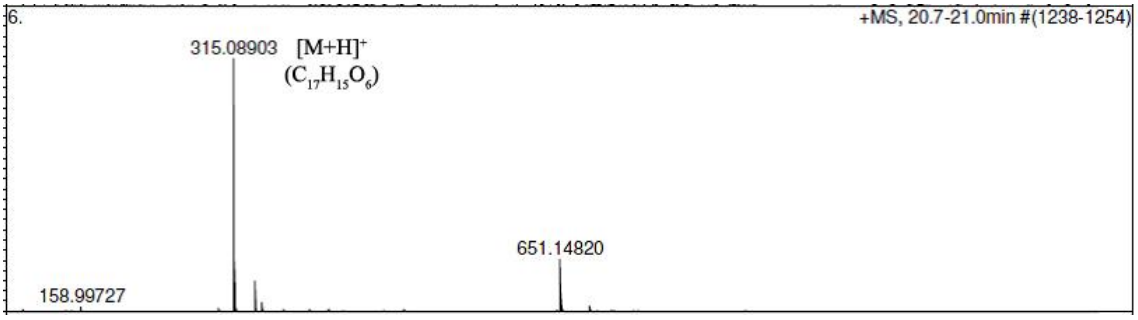

Figure S9. ESI mass spectrum obtained in the positive ion mode for compound **5**.

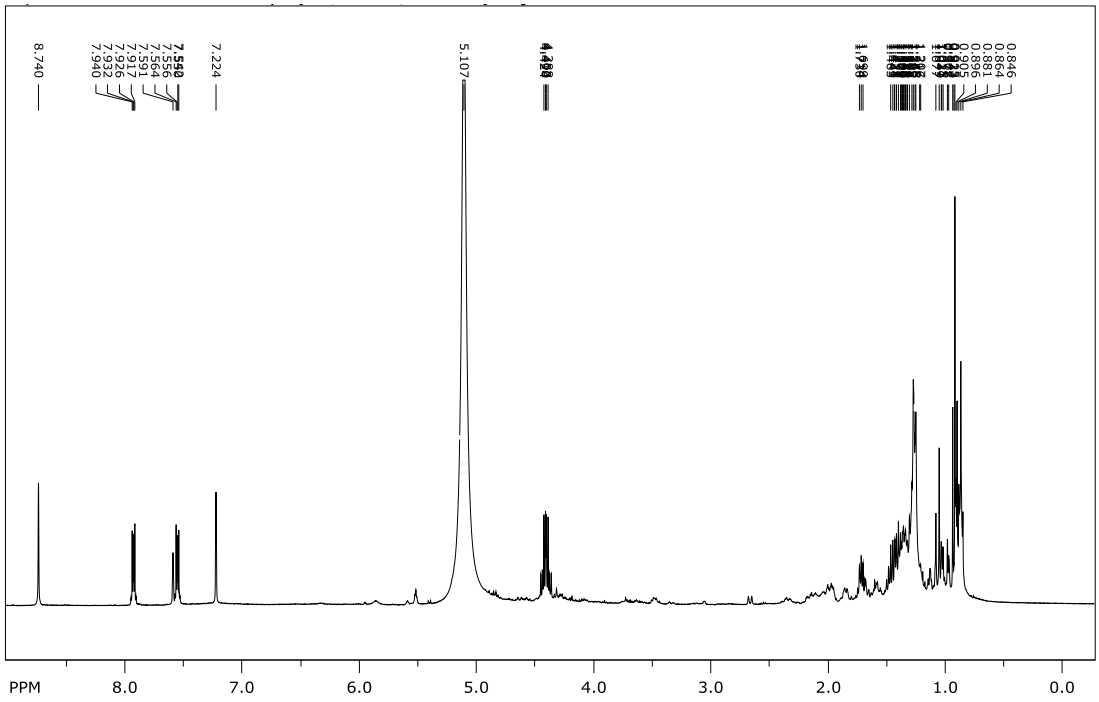

Figure S10. ^{1}H NMR spectrum (400 MHz, C_5D_5N) of compound **6**.

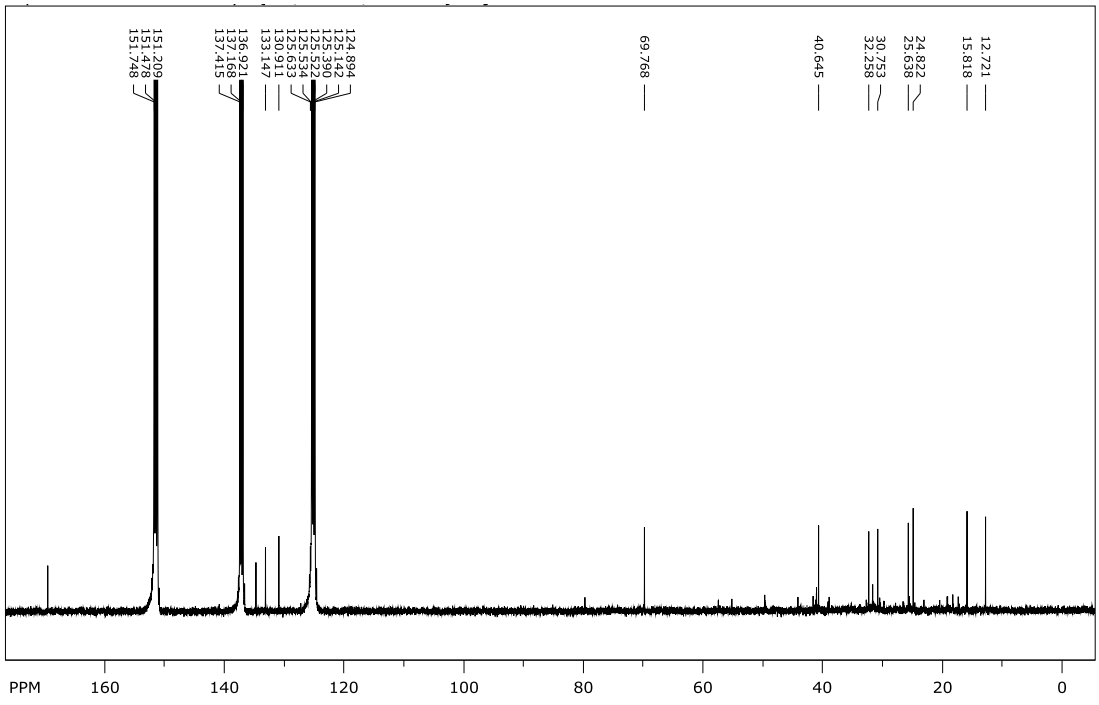

Figure S11. ^{13}C NMR spectrum (100 MHz, C_5D_5N) of compound **6**.

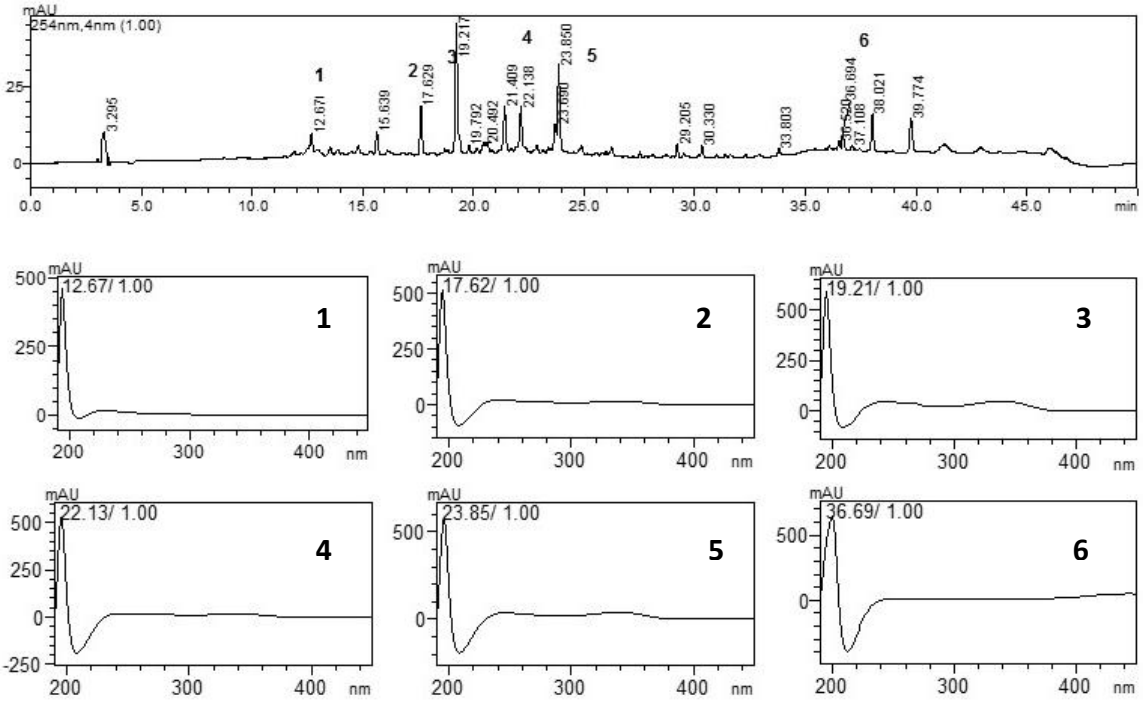

Figure S12. HPLC-DAD chromatogram of the *Vochysia divergens* extract in nature (Vd) at 254 nm and UV spectra of the compounds **1**-**6** present in the extract. Chromatographic conditions: column: Phenomenex Gemini C18 (5 µm, 250 × 4.60 mm); mobile phase: a linear gradient $CH_3OH/H_2O/CH_3COOH$ (5:94.9:0.1 v/v/v) to 100% methanol for 30 min, 100% methanol for 10 min, oven 40 °C, flow 1.0 mL min^{-1}, and a 10 µL injection volume; analysis time: 60 min, including returning to the initial condition and equilibration.

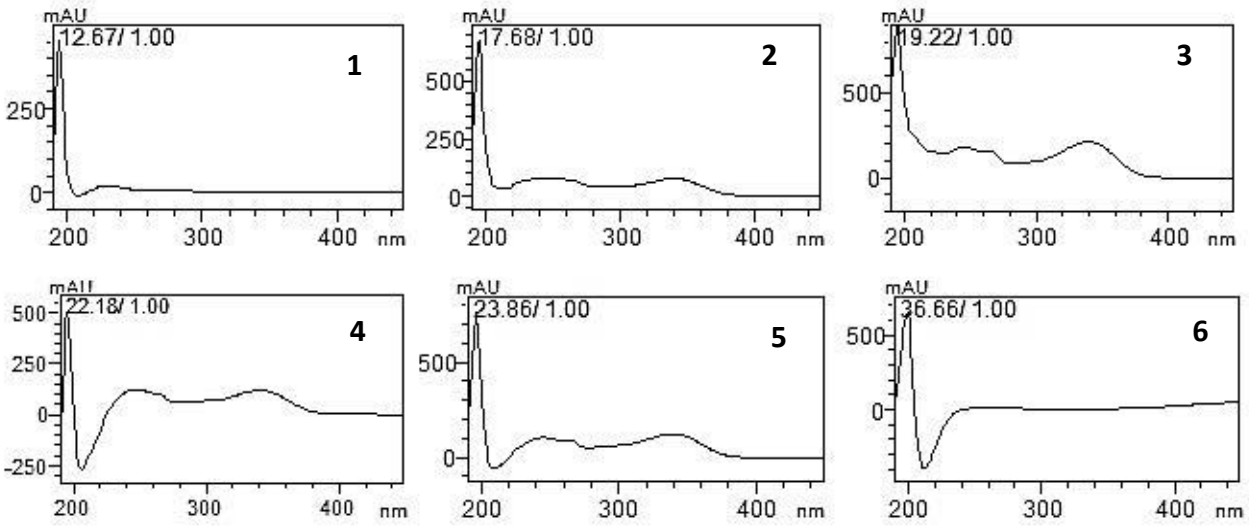

Figure S13. UV spectra of the standard compounds **1**-**6**.