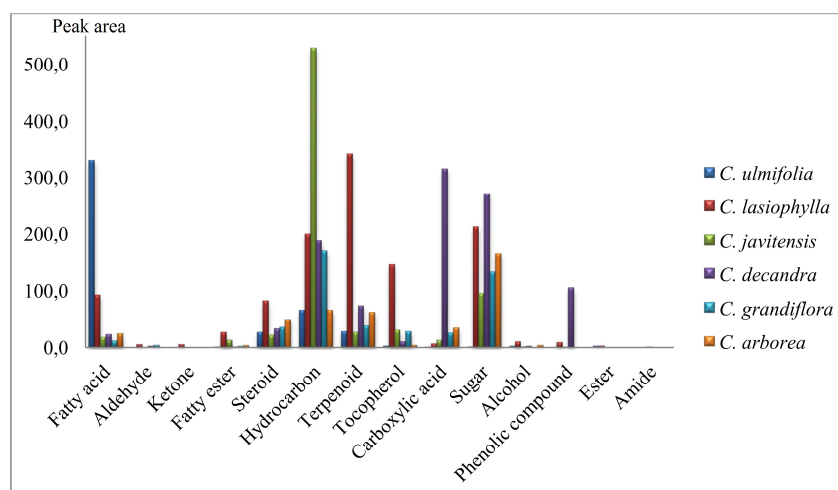


DEREPLICATION OF METABOLITES IN SIX SPECIES FROM CASEARIA GENUS USING GC-MS

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Abstract: The *Casearia* genus is widely known by the medicinal use of its species and their economical relevance. Chemically, they accumulate several substances such as flavonoids, steroids, phenolic compounds and terpenoids which are responsible for the biological activities described for those species [1]. However, some of them as well as *C. decandra*, *C. lasiophylla*, *C. arborea*, *C. javitensis*, *C. grandiflora*, *C. ulmifolia* are poorly studied from a chemical point of view. Thus, the present work proposes the identification, through Retention Index calculation and Mass Spectra similarity, of the hexanic and aqueous extracts of these six species which were analysed by GC-MS. First of all, about 10 mg of the hexanic extract were homogenized in the same solvent for the direct analysis and 5 mg were homogenized in MSTFA and pyridine for derivatization. In this method, the samples were heated at 37°C for 30 minutes. Then, they were filtrated with microfilter 0.22 µm and transferred to a 2 mL vial. The samples rested for 24 h at 5 °C and finally, 1.0 µL was injected in a gas chromatograph coupled with mass spectrometer both Shimadzu using a capillary column Agilent DB-5MS (30 m x 0.25 cm x 0.25 mm). The column oven temperature rose from 100 °C (3 minutes) to 310 °C (20 minutes) in a rate of 3 °C/min. The injection temperature was 260 °C and the mode was split (1/20). The carrier gas was helium (99.999 %) and the column flow was 1.3 mL/min. Before the silylated process, the aqueous extracts were submitted to methoximation with 20.5 mg/mL of methoxyamine hydrochloride and then heated at 30 °C for 90 minutes. Some substances are noteworthy due to their high content in such species. The graph below represents the composition which is mainly hydrocarbons (29 %), sugars (21 %), terpenoids (14 %), fatty acids (12 %) and carboxylic acids (9 %) and many of them are from metabolic pathways such as fatty acids and terpenoid biosyntheses, glycolysis, biosynthesis of plant secondary metabolites, among others. The analysis enabled the identification of several metabolites being some of them already reported in previous studies. However, many of them are being described for the first time in species from *Casearia* genus. This scientific initiation scholarship is funded by FAPESP (# 2014/02738-0).



References:

[1] Xia, L., Guo, Q., Tu, P. and Chai, X. 2014. The genus *Casearia*: a phytochemical and pharmacological overview. *Phytochemistry Reviews*. 14: 99-135.