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CHROMATOGRAPHY-FREE DEREPLICATION OF *MAYTENUS* SPP. (CELASTRACEAE) BIOACTIVE ROOT BARK EXTRACTS

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Purpose of study: Chemodiversity occurs due to the secondary metabolism of the living organisms. Natural Products scientists use structural elucidation to unveil it's diversity. Dereplication aims to optimize the time employed in this task. Hyphenated techniques, are the most used dereplication tools despite its downsides. Our present abstract used literature data to create exclusive channels of detection for bioactive quinone methide triterpenes and sesquiterpene pyridine alkaloids from root bark extracts. We based our purpose on combining ^{1}H, COSY and TOCSY NMR data acquisition to determine presence or absence. We aimed to furnish a case of raw extract dereplication success, as previously reported [1].
Methods: *ex situ* roots samples of *Maytenus ilicifolia* [**1d** = Prof. Luiz Vitor Silva do Sacramento collection in Araraquara (GPS S: -21.814885, W: -48.201091); **1c** = Prof. Ana Maria Soares Pereira collection in Ribeirão Preto (GPS S: -21.199312, W: -47.778517)] and *Maytenus gonoclada* [**1b** = preserved alive in the campus of Unesp Rio Claro (GPS S: -22.665264, W: -47.911894)] were accessed. Organic extracts [hexane: ethyl acetate (8:2)] were yielded. Shifts of quinonemethide triterpene function at position 1, 6 and 7 in rings A and B of quinonemethide triterpene were sought. In addition the isolated spin system from positions 4, 5 and 6 of pyridin protons from alkaloids had their signals monitored.

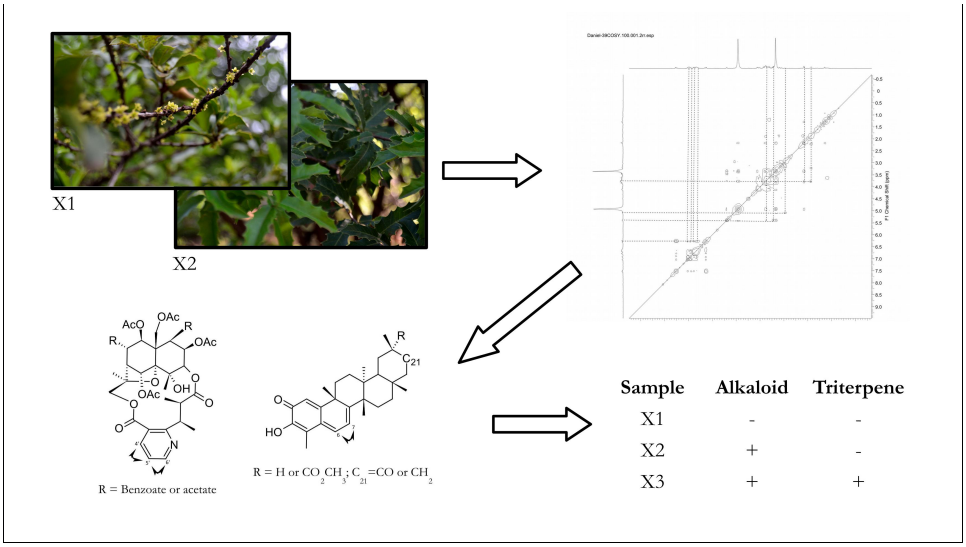

Figure1. Present paper workflow

Results: In a glance, it must be said that ^{1}H shifts of quinonemethide triterpene functions were detected in **1b** and **1c**. ^{1}H shifts of pyridin were not detectable at all probably due to the age of plants. Sample **1d** were unable to furnish high resolution spectra. COSY results did not reach diagnose of any sought metabolite's class. TOCSY isolated irridiation of doublet signals at δ 6,98 and 6,31 did confirm the presence of quinonemethide triterpene derivatives in **1b** and **1c**.
Conclusions: Our results confirmed quinonemethide triterpene deriatives within raw extracts from *Maytenus ilicifolia* and *Maytenus gonoclada*. Our chromatography-free approach might be useful for faster and "greener" dereplication of *Maytenus*' root bark. Futhermore, we will rely on this method to dereplicate extracts from different wild type *Maytenus* spp.
References: [1] Stessman, C.C., Ebel, R., Corvino, A.J., Crews, P. 2002. Employing Dereplication and Gradient 1D NMR Methods to Rapidly Characterize Sponge-Derived Sesterterpenes. J. Nat. Prod., 65, 1183–1186