5th BCNP Brazilian Conference on Natural Products
XXXI RESEM
Atibaia – SP – Brazil
ISBN: 978-85-66836-10-3
Oct. 26–29th 2015

HPLC-MS based metabolomics, dereplication and biological activities of *Byrsonima* species

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The use of analytical techniques, metabolomic tools and dereplication have increased in the field of natural products, making it possible to distinguish new compounds from those already described in complex matrixes [1] and allowing to increase the number of studied organisms and compounds identified in short time. These new analytical methods have been shown to be very useful for identification of all metabolites of plant species, and thus, for accurate studies on plant function, ecology and bio-discovery. *Byrsonima* is the largest genus belonging to the Malpighiaceae family, a tropical taxon occurring in the most part of Brazil, and known for its antimicrobial activity. This genus comprises species of medicinal importance, ornamental plants, and producers of edible fruits [2]. This research involves the evaluation of antioxidant activity by $DPPH^{\cdot}$, $ABTS^{+\cdot}$ and pyranine-based [3] methods of six extracts from different species of *Byrsonima* (*B. intermedia, B. coccolobifolia, B. verbascifolia and B. sericea*). The most active extracts were fractioned and those that presented higher antioxidant activity were subjected to HPLC-DAD-MS for tentative identification of all metabolites, including those responsible for the activity. The extracts were prepared with solvents of increasing polarity (hexane, ethyl acetate and methanol), and the methanolic extracts were subjected to bioassays and chromatographic analysis (HPLC-DAD). A bioguided-fractionation in micro scale was performed for the most active extracts in C18 cartridges using methanol:water as elution solvents in the proportions from 20:80 to 100:0 v/v. All methanolic extracts showed antioxidant capacity when compared to the standards rutin and gallic acid, and the scavenging effects obtained for $DPPH^{\cdot}$ and $ABTS^{+\cdot}$ assays ranged from 9.42 to 19.50 μg mL^{-1}, and from 2.99 to 4.43 μg mL^{-1}, respectively. The EC_{50} for pyranine-based test varied between 1.39 and 2.11 μg mL^{-1}. The fractions that presented the highest activity eluted between 40 and 50% MeOH. HPLC-DAD-ESI/MS/MS were done for these fractions using negative mode, and the molecular masses, together with the fragmentation patterns and data from literature, allowed to tentative identify gallic acid and gallic acid derivatives, pentosides and hexosides of quercetin and proanthocyanidin dimmers and trimmers, classes of secondary metabolites known to exhibit a high antioxidant activity.

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Acknowledgements: FAPESP