



***Virola* PLANTS FROM COLOMBIAN AMAZON: LC-HRMS, ¹H-RMN, AND GC-MS-BASED CHEMICAL PROFILING AND ANTIFUNGAL ACTIVITY**

Luisa L. Orduz-Diaz¹, Luis E. Cuca¹, Lydia F. Yamaguchi², Massuo J. Kato², Ericsson Coy-Barrera³

¹ Department of Chemistry, Universidad Nacional de Colombia, Bogotá, Colombia, ² Institute of Chemistry, Universidade de São Paulo, São Paulo- Brasil. ³ Faculty of Basic and Applied Science, Universidad Militar Nueva Granada, AA 49300, Cajicá, Colombia.

Abstract: In the search for antifungal bioactives, natural extracts are a promising opportunity. Plants belonging to the genus *Virola* are widely used by indigenous communities in the Colombian Amazon due to their medicinal properties, *Virola* is one of the most important genera of the Myristicaceae family; in Colombia, twenty one species can be found. [1], and they have also been reported as potential antifungals [2,3,4]. Twenty eight ethanol-soluble extracts from different plant parts (leaves, wood, bark, flowers and fruits) belonging to the genus *Virola* (*V. carinata*, *V. elongata*, *V. peruviana*, and *V. callophylla*) and twelve fractions were evaluated using a micro-scale amended medium method against *Fusarium oxysporum*, the causal agent of vascular wilt disease in plants of economic importance such as tomato (*Solanum lycopersicum*), banana (*Musa paradisiaca*) and carnation (*Dianthus caryophyllus*). The extracts were profiled using LC-HRMS and ¹H-RMN techniques, and the *n*-hexane-soluble fraction of the extracts was analyzed by GC-MS. The antifungal activity of the extracts was determined at three concentrations finding inhibition values higher than 90%. The results indicated that extracts exhibited dose-dependent inhibition of fungal mycelium at different levels. The analysis of chromatographic/spectroscopic data indicated the presence of particular compounds in some extracts such as flavonoids which was confirmed by a comparative study with some isolated compounds within a derreplicative process. A multivariate analysis by principal component analysis (PCA) of the complete chromatographic and spectroscopic data profiles showed some clusters. This clustering confirmed the similarity of extracts of the same plant, even in the composition of extracts of bark and most wood plants, which would not be just possible with direct comparison of the chromatographic/spectroscopic data. The correlation between the antifungal activity (as supervision variable) and chromatographic/spectroscopic data was performed through Partial Least Squares (PLS). This analysis allowed finding some groups of signals having high correlation with the activity which were tentatively identified by HRMS. The present protocol let to the discrimination of active extracts within a rational searching of antifungals from *Virola* species. *The present work is a product derived by the Project INV-CIAS-1788 financed by Vicerrectoría de Investigaciones at UMNG - Validity 2015.*

References

- [1] Shultes, R. E.; Hofmann, A.; Rälsh, C, 2000. Plantas de los Dioses. Las fuerzas mágicas de las plantas alucinógenas; Fondo de Cultura Económica: México, p 176.
- [2]. Lopes, N.P., Kato, M.J., Yoshida, M., 1999. Antifungal constituents from roots of *Virola surinamensis*. *Phytochemistry*, 51(1): p. 29-33.
- [3] Sartorelli, P., Young M.C.M., Kato, M.J, 1998. Antifungal lignans from the arils of *Virola oleifera*. *Phytochemistry*, 47(6): p. 1003-1006.
- [4] Zacchino, S., Rodríguez, G, Santecchia, C., Pezzenati, G., Giannini, F., Enriz, R. 1998. *In vitro* studies on mode of action of antifungal 8.O.4'-neolignans occurring in certain species of *Virola* and related genera of Myristicaceae. *Journal of Ethnopharmacology*, 62(1): p. 35-41.