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Principal component analysis (PCA) of ^{1}H NMR and antifungal assay of *Hedyosmum brasiliense* male and female extracts from Cerrado and Atlantic Forest

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Hedyosmum brasiliense is a dioecious shrub from Chloranthaceae, widely distributed in Central, Southeastern and Southern Brazilian regions. The aim of this work was to investigate the difference among male and female crude extracts of *H. brasiliense* obtained from Cerrado and Atlantic Forest using multivariate analysis and its antifungal activity. Ethanolic extracts were prepared from leaves of male and female plants of each biome and 5.0 mg of each extract were lyophilized in triplicate, diluted in 700 μL of $CDCl_3$ and transferred to 5 mm glass tubes. A total of 12 samples were analyzed by Hydrogen Nuclear Magnetic Resonance (^{1}H NMR 600 MHz). All spectra baselines were adjusted and chemical shifts were referenced by tetramethylsilane (TMS) signals. Regions corresponding to TMS and $CDCl_3$ of all spectra were suppressed. PCA was executed by NIPALS method using Matlab®. For antifungal assay by bioautography, 400 μg of each extract and 5 μg of nystatin were applied in TLC silica gel 60 F^{254}, developed with chloroform/acetone (6:1) and registered at (λ) 254 and 366 nm. Suspensions of *Cladosporium cladosporioides* and *C. sphaerospermum* fungi were sprayed over the plates and incubated for 48 h. Both Atlantic Forest extracts presented strong antifungal activity at Retention Factor (Rf) from 0.53 to 0.67 while those from Cerrado were inactive at the same Rf, suggesting that male and female extracts are chemically similar and the environmental conditions influenced on the biosynthesis of secondary metabolites in this species. However, comparing all extracts by PCA of the ^{1}H NMR fingerprinting spectrum, it was possible to discriminate Cerrado and Atlantic Forest extracts with 99% of explained variance by PC1 x PC2, attributing most of the difference to the signal at δ 1.25 in the NMR spectra. This simple, quick and effective method for crude extract analysis allowed confirming the chemical difference between Cerrado and Atlantic Forest extracts by their antifungal activity and metabolomics.

Keywords: dioecy, ^{1}H NMR, antifungal, Cerrado, Atlantic Forest.

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