

# The 1st International Electronic Conference on Medicinal Chemistry and Pharmaceutics



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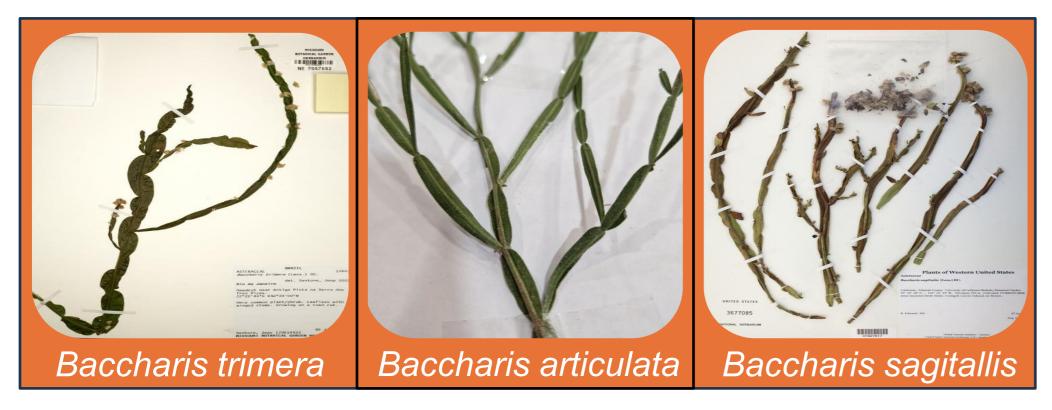
# Chemometric Multivariate Analysis for Species Classification in the Genus Baccharis (Asteraceae)

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# **INTRODUCTION & AIM**

Carquejas (*Baccharis* spp.) are among the ten most traded medicinal plants in Brazil. Despite their popularity, only *Baccharis* trimera has an official quality control protocol, which is restricted to morphological characteristics.



This study developed a machine learning—based chemometric model using mid-infrared Fourier Transform Infrared Spectroscopy (FTIR) and multivariate analysis to improve species authentication and strengthen quality control of commercial *carqueja* products.

**METHOD** 

#### Baccharis trimera; Plant species Baccharis articulata; acqusition and Baccharis sagittalis; processing Baccharis junciformis; Baccharis pentaptera; **MIR-FTIR** Hydroalcoholic spectral extracts: acquisition 50 spectra per species MIR-FTIR Hydroalcoholic Complete dataset extracts: 250 spectra in total SNV Mean Center Data preprocessing Smoothing Multivariate analysis Dataset split: Unsupervised Supervised 70% calibration analysis analysis 30% validation **MATLAB** Feature

PLS-DA

Plant species

discrimination

importance

analysis (VIP)

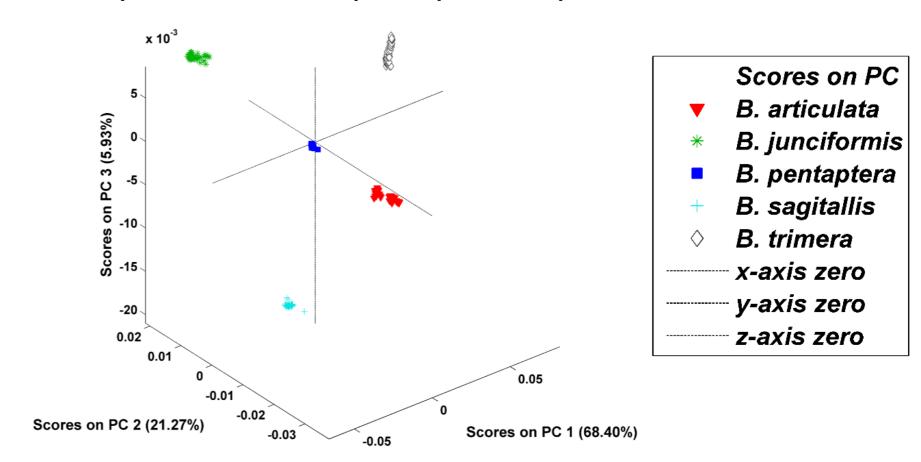
**PCA** 

Plant species

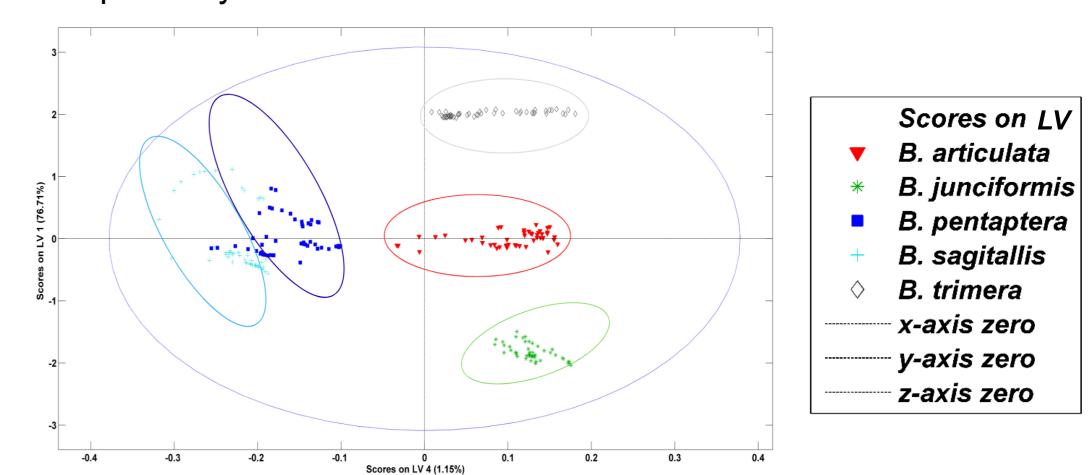
identification

## **RESULTS & DISCUSSION**

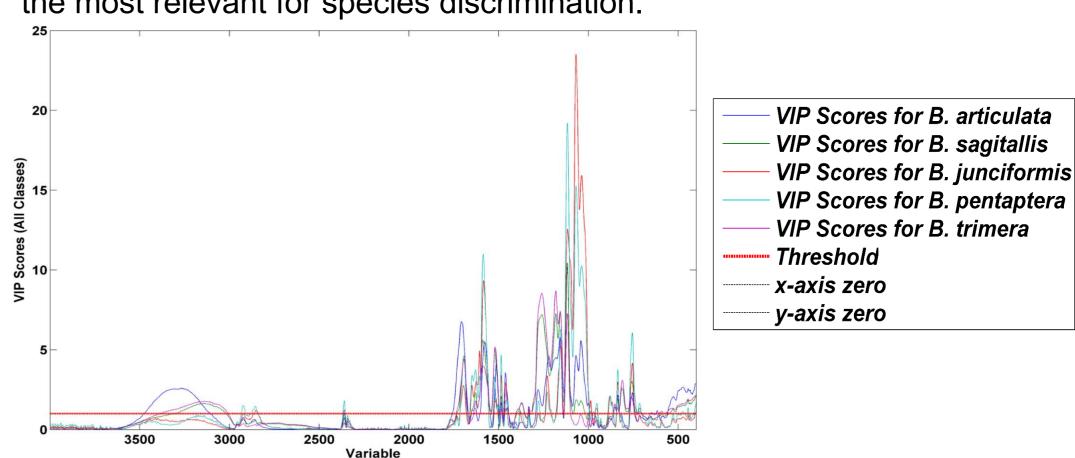
PCA captured 98% of total variance, clearly discriminating all five *Baccharis* species with six principal components.



The PLS-DA model explained 88.9% of the total variance. Using four latent variables, the model achieved 90% overall classification accuracy, with specificity and sensitivity of 90%. and 71%, respectively.



The spectral regions between 1750 and 750 cm<sup>-1</sup> were identified as the most relevant for species discrimination.



### CONCLUSION

Machine learning-based chemometric models successfully distinguished the *Baccharis* species, reinforcing their value as innovative tools for quality control and standardization of carqueja products.

# FUTURE WORK / REFERENCES

