

# 1st International Electronic Conference on Metabolomics

1-30 November 2016  
chaired by Dr. Peter Meikle

sponsored by



metabolites

## Metabolomic to target insecticidal compounds of *Caesalpinia pluviosa* var. *peltophoroides* against *Spodoptera frugiperda*

João Luiz Baldim Zanin<sup>1</sup>, Olivia Silva Domingos<sup>1</sup>, Antônio Rogério Bernardo<sup>2</sup>, Ana Carolina Volante<sup>2</sup>, Andréia Pereira Matos<sup>2</sup>, João Henrique Ghilardi Lago<sup>3</sup>, Daniela Aparecida Chagas-Paula<sup>1,\*</sup>, Marisi Gomes Soares<sup>1</sup>

<sup>1</sup> Laboratório de Fitoquímica e Química Medicinal - LFQM, Instituto de Química, Universidade Federal de Alfenas – UNIFAL-MG, Alfenas - MG.

<sup>2</sup> Departamento de Ciências Exatas, Universidade Federal de São Carlos - UFSCar, São Carlos - SP.

<sup>3</sup> Departamento de Ciências Exatas e da Terra, Universidade Federal de São Paulo - UNIFESP, São Paulo - SP.

\* Corresponding author: [da.chagaspaula@gmail.com](mailto:da.chagaspaula@gmail.com)





## Abstract

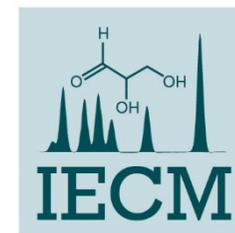
**Introduction:** *Spodoptera frugiperda* (Lepidoptera: Noctuidae) is one of the main plagues of maize cultivation and it is resistant to the most used insecticides. Plants are important source of biopesticides due to their own mechanisms of interaction and diversified composition. Thus, fractions (hexane, acetate and hydro-ethanol ) of extracts from different parts of *Caesalpinia pluviosa* var. *peltophoroides* (Fabaceae) have their insecticidal activity investigated. Chemical composition of fractions were evaluated by UHPLC-HRFTMS, thereafter processed on MZmine 2.2 software and exported to do multivariate statistical analysis (MSA) - O2PLS-DA (SIMCA-P 13.0). The dereplication of compounds were performed using DNP<sup>®</sup> , Scifinder<sup>®</sup> and our in house *Caesalpinia* database.

**Results and Discussion:** Six fractions were inactive and five displayed pupal or larval mortality. The O2PLS-DA analysis found a clear separation of inactive and insecticidal group ( $R^2= 0,72$ ) and indicated the metabolites highly correlated with the insecticidal property ( $VIP>1.95$ ): eugenyl vicianoside; gluconic acid lactone and gallic acid.

**Conclusions:** Through metabolomic strategies was possible to dereplicate the compounds most correlated with insecticidal property and this knowledge can be very useful to development of new techniques to the crop pest control.

Acknowledgements: FAPEMIG and CNPQ for the financial funding and the AsterBioChem for the UHPLC-HRMS analysis.

**Keywords:** metabolomic; *Caesalpinia pluviosa*; *Spodoptera frugiperda*; insecticidal; UHPLC-HRMS



# Introduction

-*Spodoptera frugiperda* (Lepidoptera: Noctuidae) is one of the main plagues of maize cultivation.



Source: [www.agrolink.com.br](http://www.agrolink.com.br)

-It is resistant to the most used insecticides only controlled with pyrethroids and organophosphates (RIBEIRO et al., 2012).



Source: <http://www.pioneersementes.com.br>

-Plants are important source of biopesticides due to the diversified occurrence of secondary metabolites and the evolution of natural mechanisms of interaction (defense or attraction).



# Introduction



*Caesalpinia pluviosa* var. *peltophoroides* (Fabaceae)



Flowers

Leaves

Fruits

Stem bark



Extracts



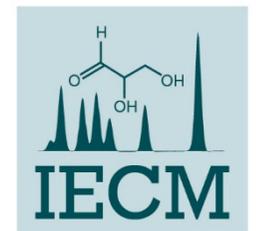
Fractions

Hexane

Ethyl acetate

Hydro-ethanol

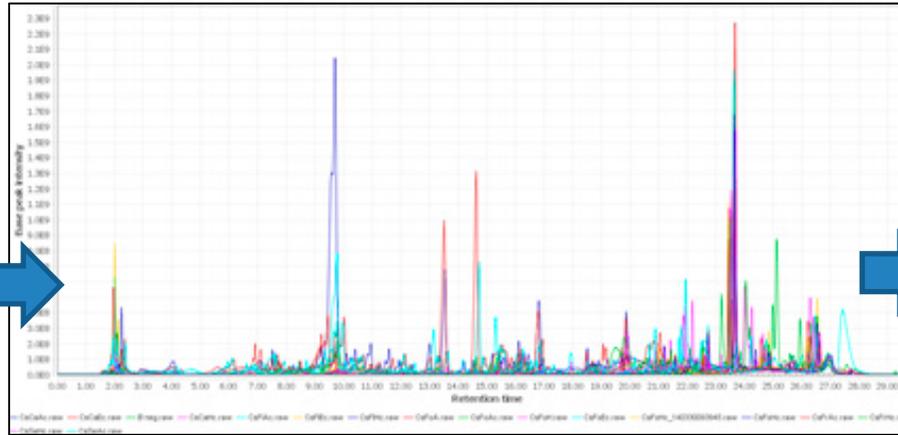
All fractions have their *in vitro* insecticidal activity investigated against *Spodoptera frugiperda*



# Introduction



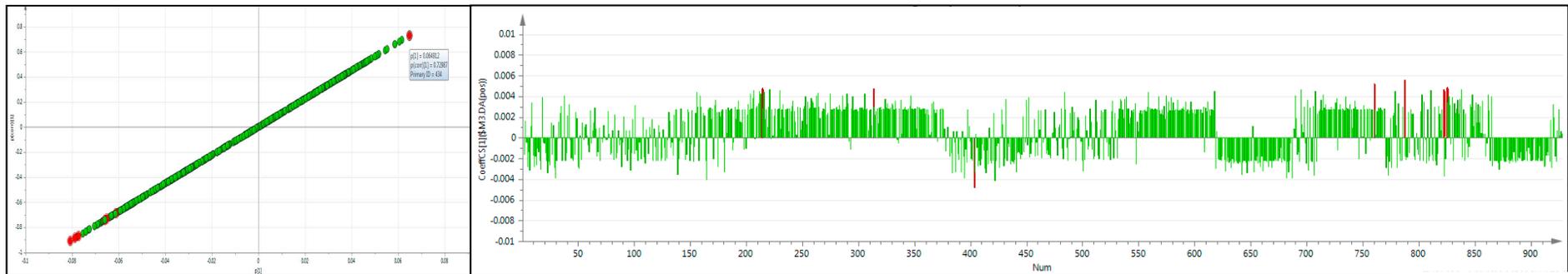
Chemical composition  
evaluated by  
UHPLC-HRFTMS



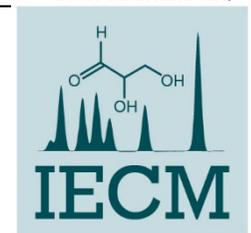
Data treatment on  
MZmine 2.2 software

Multivariate statistical analysis  
O2PLS-DA on SIMCA-P 13.0 software

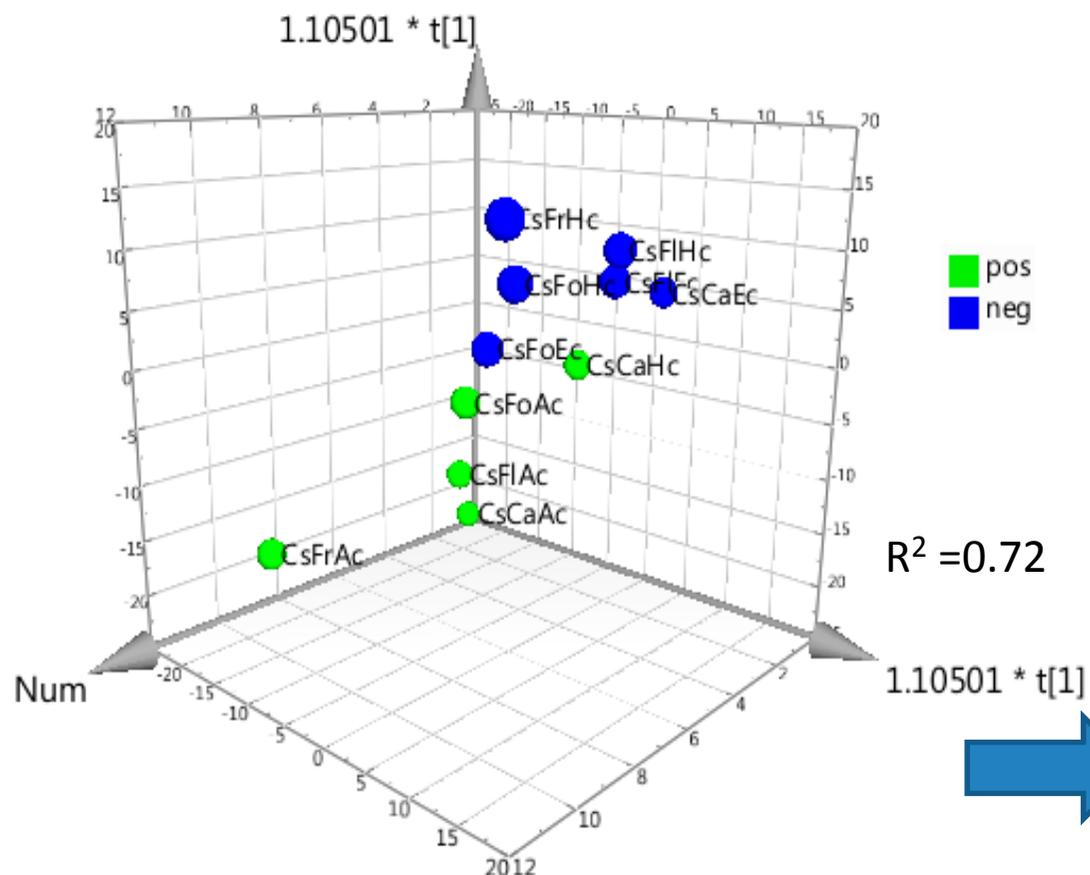
Determination of compounds correlated to the insecticidal activity



Dereplication using DNP<sup>®</sup>, Scifinder<sup>®</sup> and our in house *Caesalpinia* database



# Results and Discussion

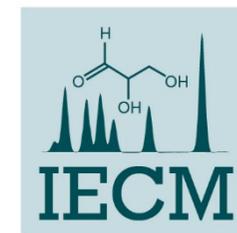


-Six fractions were inactive and five displayed pupal or larval mortality;

-The O2PLS-DA analysis found a clear separation of inactive and insecticidal group;

**Indicating the most important variables in the projection (VIP > 1.9).**

Retention time	[M-H] <sup>-</sup>	Molecular formula	Error (ppm)	Dereplication	VIP
6.98	457.1709	C <sub>21</sub> H <sub>30</sub> O <sub>11</sub>	-1,17	Eugenyl vicinoside	2.2
2.20	177.0395	C <sub>6</sub> H <sub>10</sub> O <sub>6</sub>	-5,43	Gluconic acid lactone	2.1
4.17	169.0133	C <sub>7</sub> H <sub>6</sub> O <sub>5</sub>	-5,6	Gallic acid	1.9



## Conclusion

-Through metabolomic strategies was possible to dereplicate the compounds most correlated with insecticidal property

-The fractions and substances correlate with this property can be very useful to development of new techniques to the crop pest control.



# Acknowledgements

Financial support:



UHPLC-MS analysis:



Metabolomic studies

