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Testing the suitability of preserved insect collections for bio-discovery using liquid chromatography mass spectrometry

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Abstract:

Small metabolites and venom metabolites produced by insects are known to exhibit biological activity. These metabolites could be used to develop natural product-based therapeutics. To screen for these metabolites, insects must be collected and accurately identified. Natural history collections consist of identified insects and provide a source of raw material for metabolomic screening. The objective of this research was to understand whether preservation significantly altered the insect metabolomic profiles. Insects from the family Sphecidae: *Podalonia tydei* (Le Guillou), which were preserved in ethanol and flash frozen, were homogenized with methanol. The resulting metabolomic extracts and storage ethanol were analysed using untargeted liquid chromatography-mass spectrometry. Mass spectral data were processed with MZmine2. The data were analysed using multivariate statistical analysis. In the Principal Component Analysis, ethanol stored samples and their storage solvents clustered close together and this was verified by Analysis of Similarity (ANOSIM). Based on ANOSIM (p = 0.003, R2= 0.48) there was significant overlap between chemical profiles of treatments (ethanol only, ethanol stored tissue, flash frozen tissue). A group of acyl-carnitines were putatively identified from the extracts. The flash frozen samples have a high relative abundance for acyl-carnitines, however the Kruskal Wallis (p > 0.05) showed no significant difference between the median of abundance. Therefore, preserved insects from natural history collections and their ethanol storage solvents could be used for metabolomic screening. However, it would be best to use specimens from the same species preserved under various conditions to capture metabolites that may degrade or leach during preservation.

Keywords: Preserved collections; Biodiscovery; Metabolomics; Hymenoptera

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Introduction

- Natural products remerging as drug candidates
- Fast and efficient screening required (chromatography-mass spectrometry)
- Potential to use preserved collections

 -accurately identified sources
 -many species under the same roof
- Australian National Insect collection bees and wasps are suitable candidates -antimicrobial compounds (e.g. apidaecin type peptides)



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Introduction

Screening pipeline

Metabolomic extracts

(insects preserved under different conditions)

Liquid Chromatography tandem mass spectrometry (LC-MS/MS)

Mass spectral data processing

(MZmine 2)

Descriptive statical analysis

(PCA, ANOSIM, UpSet plot, Boxplot)

Results and discussion



Fig.1. PCA score plot for metabolomic profiles of frozen tissue, ethanol stored tissue & ethanol extracts

Significant but low overlap between the chemical profiles of different treatments (PC1 & PC2 ANOSIM, $R^2 0.48$, p = 0.003)

Results and discussion



Fig.2. Boxplot for putatively identified acyl-carnitines from frozen tissue, ethanol stored tissue & ethanol extracts no significant difference between acyl-carnitines or other putatively identified metabolites



Results and discussion



Fig.3. Upset plot for the amount of overlap between treatments (frozen tissue, ethanol stored tissue, storage ethanol)

Conclusions

- There is an overlap between chemical profiles of preserved vs fresh insects
- Preserved collections including storage solvents could be used for the initial screening of small metabolites during biodiscovery
- This potentially eliminates the time taken for sampling, and identification and supports natural product drug discovery



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