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PSB-META-05 / Metabolomics and dereplication study of the British Bluebell

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Introduction

Metabolomics is the technology designed to provide general qualitative and quantitative profile of metabolites in organisms exposed to different conditions. Metabolomics is applied in many aspects of natural drug discoveries, particularly in bioactivity screening to improve dereplication and identification procedures. Fast dereplication of known compounds and identification of lead bioactive metabolites is important in the primary stages of metabolomics profiling prior to an intensive isolation work.

Methods

Two levels of metabolomics were used in this study. First was metabolites fingerprinting which aimed for rapid classification of samples by comparing the metabolites patterns or fingerprints. Second was metabolites profiling and dereplication study for the secondary metabolites related to a specific pathway in order to individually identify and quantify these metabolites.

Results

British Bluebell was collected at different times of the year, extracted and subjected to HR-MS and NMR analysis. NMR data were used to compare the metabolites pattern between the extracts. Metabolomic profiling and dereplication studies, using HR-MS were done for different extracts in order to highlight the seasonal variation in production of secondary metabolites. Dereplication studies were accomplished by utilizing the MZmine 2.10 software with aid of DNP databases. Multivariate data analysis was employed by using PCA in order to classify samples into groups, trends and outliers, which maximize the information, can be obtained from spectral data. OPLS-DA was used to correlate the chemical profile with tested biological activity. Metabolomics has been shown to be a powerful tool in highlighting the seasonal variation in the metabolites produced by the British BlueBell.[1, 2, 3, 4]

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Novel Aspect

Using Metabolomics as a tool to enhance natural products drug discovery

Keywords

Metabolomics, Dereplication, Profiling, Bluebell, metabolites fingerprinting, multivariate data analysis