Analysis of Metabolites from Solanum Species using Gas Chromatography-Time Of Flight Mass Spectrometry and Automated Data Analysis


We acknowledge the support of the Food Standards Agency and the Scottish Executive Environment and Rural Affairs Department.

We have developed a metabolite profiling technique based on Xcalibur™ software programmes. Analysis of metabolites from Solanum species using gas chromatography-time of flight mass spectrometry is a useful tool for the study of metabolite distribution within plant populations. Having selected ion(s) suitable for detection of each component, a time window is defined for each component relative to an adjacent retention standard.

Inositol (IS)

Separate layers (centrifuge) no heat or vacuum (3) CHCl₃ (+) + fructose 1 split 167:1

Inositol

Fructose

Relative Abundance

Retention Standards

Feature All Some Purpose

1 Analytical Blank

2 Reference standard

4 Multiple extracts

5 Two split levels

10 Instrumental reproducibility during sequence (check for drift)

Statistical treatment of data eg: ANOVA
• Principal Components
• Similarity
• Response ratios

Comparison of mass spectra of analytes with entries in the NIST mass spectral library.

The profiling technique is being used to measure metabolite variation within Solanum germplasm collections in an attempt to relate metabolite distribution to phenotypic characteristics and to look for phytochemical diversity.