Comparing the Effects of Different Management Practices on the Metabolite Composition of Cereal Crops using a GC-MS based Approach

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Introduction

We are investigating the effects of conventional *vs.* integrated management practices on both the chemical composition & agronomic properties in six crop species of major economic importance in Scotland (potato, Spring & Winter barley, field beans & Winter wheat). This is being conducted using a long-term rotation, set up in 2009, at the James Hutton Institute's Centre for Sustainable Cropping (CSC*) at Balruddery Farm in Angus. For each crop one industry standard Variety was chosen, along with four others selected for optimum performance under reduced Inputs &/or for differing end use sector requirements.

*http://csc.hutton.ac.uk/

Methods

1. Metabolite Analysis

Compositional analysis of organic metabolites in each of the three cereal crops - Spring & Winter barley, & Winter wheat (grown over five consecutive Years: 2011-2015), were determined by GC-MS (Gas Chromatography-Mass Spectrometry), post-harvest (Figure 1).

2. Statistical Analyses

- Principal Components Analysis (PCA).
- Restricted Maximum Likelihood (REML).

Questions Being Asked:

- Are there differences between Varieties, Inputs & Years?
- Are any differences between Variety & Input, consistent over the five Years?
- What are the metabolic processes that drive variation?

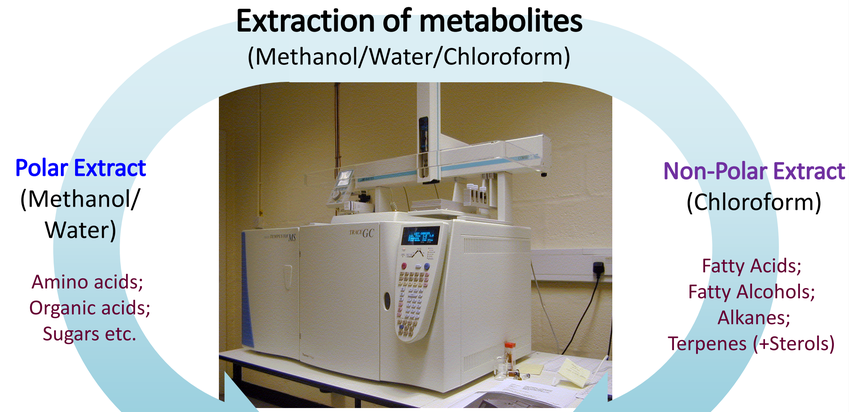


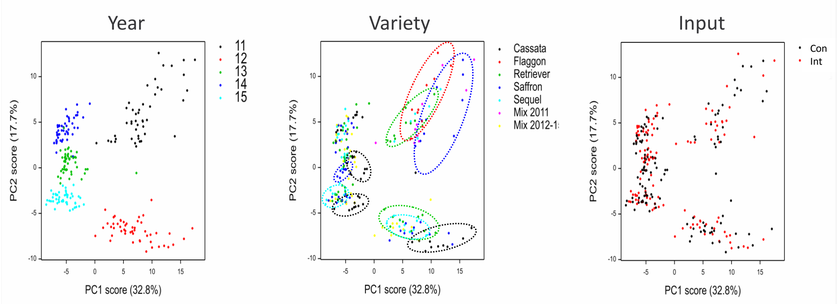
Figure 1. Extraction & Analysis of Metabolites using GC-MS

Results

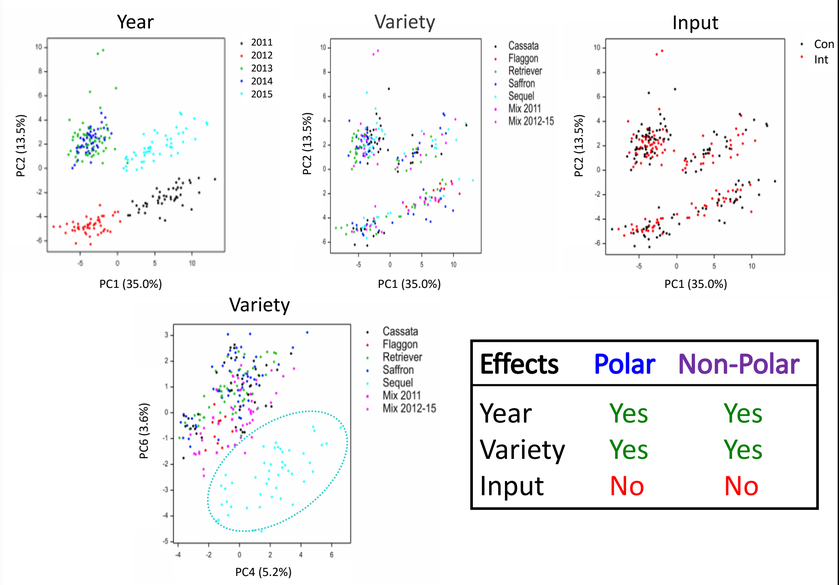
Example: Winter Barley 2011-2015:

- PCA – Looks at the 'whole picture'.
- Are distinct groups separating?

Polar Metabolites



Non-Polar Metabolites

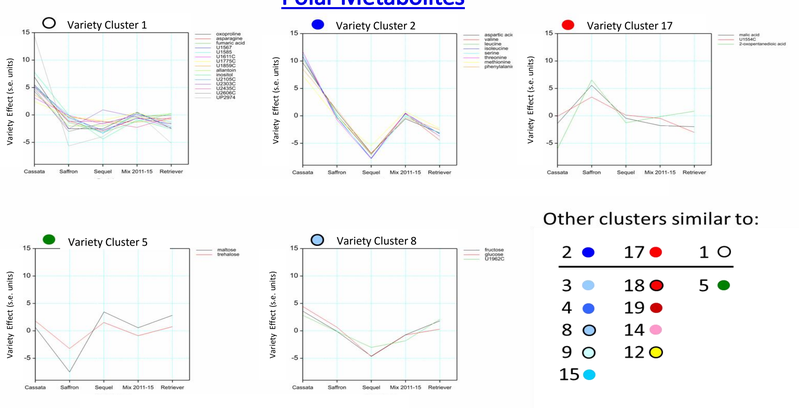


Effects	Polar	Non-Polar
Year	Yes	Yes
Variety	Yes	Yes
Input	No	No

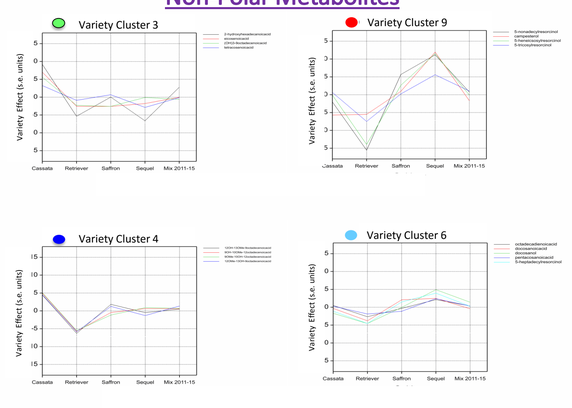
REML Over-Years Cluster Analysis (Winter Barley 2011-2015):

- Looks at similarity in patterns of inter-Variety variability.
- Are there any groupings of individual compounds that show similar patterns of inter-Variety variability over Years?

Polar Metabolites

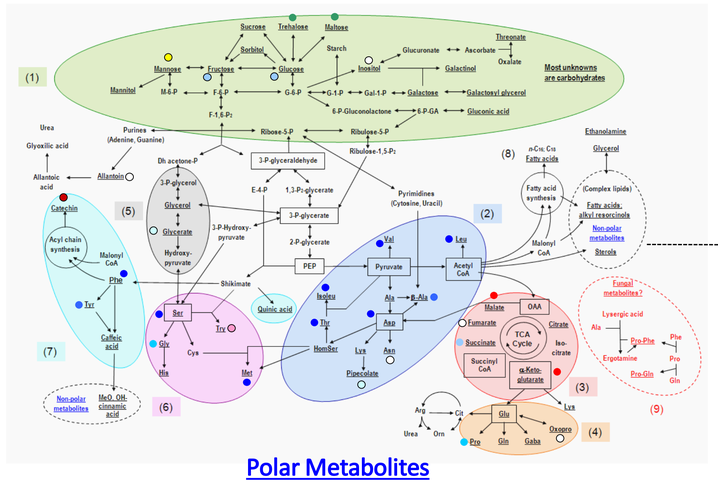


Non-Polar Metabolites

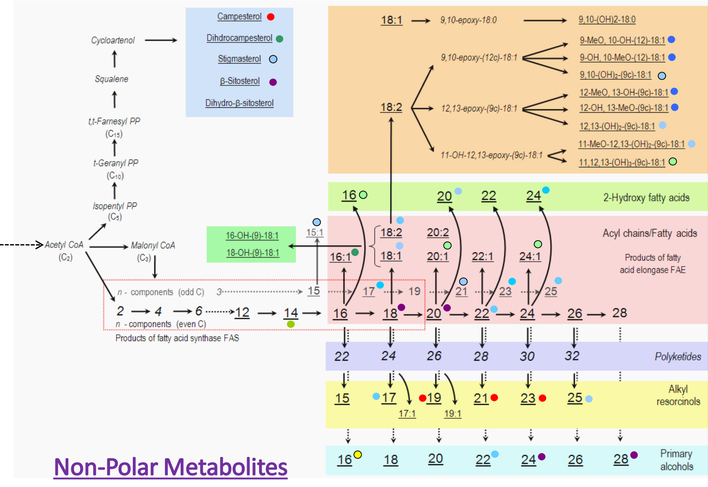


Polar Metabolites:
26 known & 25 unknown metabolites significantly different. 18 cluster groups (mainly amino acids, organic acids, carbohydrates) identified (five shown above).

Non-Polar Metabolites:
38 known metabolites significantly different. 11 cluster groups identified (four shown above).



Polar Metabolites



Non-Polar Metabolites

Conclusions

- Preliminary analyses of data for all three cereal crop types (grown over 2011-2015 of the rotation) using PCA, indicates that Year (seasonal variation) has the greatest effect on metabolite composition.
- There is also evidence for Variety-related variation in composition within individual Years.
- There may be limited evidence for Input effects. Generally, crop growth Inputs (conventional *vs.* integrated) appears to have little effect on the composition of primary metabolites in cereal grains.
- The significance of any such effects will be determined following completion of in-depth over-Years statistical analyses for all three cereal crops.

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