INTRODUCTION
Success rate in metabolomic studies largely depends on the quality of sample preparation, the stability and reproducibility of the separation and detection and quality of data handling/interpretation. The reproducibility of the sample preparation step is a critical parameter. For metabolomic profiling of biological samples using GC-MS, often a combination of oximation and silylation is used and this derivatisation method is applicable to acids (e.g. fatty acids), sterols, amines, amino acids, sugars, etc. Automation of the derivatisation process enhances repeatability and the time between sample preparation and analysis can be kept short and constant, which is important since TMS-derivatives have a limited stability. GC-MS analysis using retention time locked conditions results in stable retention times in function of time and allows comparison of large data sets, even on different (but same nominal) columns. In this study, Arabidopsis thaliana, a popular model organism in plant biology and genetics, was used for testing an automated sample preparation approach upfront GC-MS analysis. Several features that were up- or down regulated in the different species were revealed by means of PCA and ANOVA.

EXPERIMENTAL
Plant tissue samples from 2 genotypes (Wassilewskija and Columbia) and two ages (young, old) were extracted by chloroform/methanol/water. The asexual phase was dried under nitrogen. Oximation and silylation were carried out on an Agilent 7980A automatic Liquid Sampler.

RESULTS
A typical GC-MS profile obtained for the hydrophobic fraction of Arabidopsis thaliana is shown below in Figure 2.

Table 1. Automated Sample Preparation Sequence

<table>
<thead>
<tr>
<th>Step</th>
<th>Description</th>
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<tbody>
<tr>
<td>1</td>
<td>Mix 100 mg sample with 300 µL chloroform, 300 µL methanol and 200 µL water</td>
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<td>2</td>
<td>Incubate 10 min at 60 °C</td>
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<th>Data (Retention Time)</th>
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<tr>
<td>Myristic Acid (40:0)</td>
<td>7.9</td>
</tr>
<tr>
<td>2-Hexadecanone (6:0/9)</td>
<td>36.1</td>
</tr>
<tr>
<td>Phosphoric acid (9:866)</td>
<td>6.46</td>
</tr>
<tr>
<td>L-threonine 1 (10:224)</td>
<td>6.42</td>
</tr>
<tr>
<td>Rhamnose 1 (10:46)</td>
<td>5.3</td>
</tr>
<tr>
<td>Asparagine 1 (12:002)</td>
<td>2.03</td>
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<tr>
<td>D-malic acid (12:766)</td>
<td>3.3</td>
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<tr>
<td>L-glutamic acid 1 (13:138)</td>
<td>10.64</td>
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<tr>
<td>Putrescine (21:763)</td>
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<tr>
<td>Dehydroascorbic acid 1 (16:163)</td>
<td>6.96</td>
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<tr>
<td>L-ornithine 1 (27:325)</td>
<td>9.55</td>
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<tr>
<td>Methyl-beta-D-glucopyranoside</td>
<td>7.56</td>
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<tr>
<td>L-threonine 2 (10:224)</td>
<td>5.64</td>
</tr>
<tr>
<td>Glycine 1 (24:735)</td>
<td>8.64</td>
</tr>
<tr>
<td>Galactose 1 (24:444)</td>
<td>5.92</td>
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</table>

Data Analysis
Samples were processed via two strategies:

1. Data deconvolution by means of AMDIS and data preprocessing (alignment, normalization, fitting) + statistical analysis in Mass Profiler Professional (MPP)

CONCLUSIONS
Automated sample preparation results in much better reproducibility.
Detailed profiles are obtained under RTI-GC-MS conditions.
Upon analyzing different plant samples, several discriminating features could be revealed.

ACKNOWLEDGEMENT
The authors want to thank Steve Fisher (Agilent Technologies) for his support with MPP.