INCREASING THROUGHPUT EFFICIENCY LEADS TO GREATER EFFICIENCY IN JUICE QUALITY LABORATORY

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INTRODUCTION

Today, supermarket shelves showcase many different products that offer many different flavors and health properties to the consumer.

The competition within this industry is fierce with many new products entering the marketplace every year that contain new flavors or superfruits into the product.

For food and beverage manufacturers there is a need to ensure certain criteria are met for all their product portfolio:

- **Produce products that meet required internal and external safety legislation / procedures**
- **Deliver a consistent product that meets labelling requirements**
- **Satisfy consumer demand with amount of juice produced**
- **Develop and launch innovative products to support new market opportunities**

These activities require technical support—both for routine analysis and also for method development and this can place high demand onto instrument use.

In order to increase efficiency of the lab and reduce lab costs, Acquity UPLC™ was introduced and this poster illustrates one of the method developed for routine analysis.

METHODS

Sample Preparation
Each sample was diluted with water:methanol (75:25) and filtered through a 0.45 µm filter

Acquity UPLC conditions
Solvent A: Water + 0.1% Acetic acid
Solvent B: Acetonitrile + 0.1% Acetic acid
Guard column: Vanguard
Column: HSS T3, 2.1 x 100mm, 1.7um
Column temp: 45°C

Table1. UPLC Gradient

Time	Flow Rate	%A	%B	Curve
Initial	0.65	99.0	1.0	
1.00	0.65	99.0	1.0	6
17.00	0.65	60.0	40.0	6
21.00	0.65	5.0	95.0	6
22.00	0.65	99.0	1.0	6
25.00	0.65	99.0	1.0	6

Acquity TUV conditions
The UV chromatogram was used to obtain a chromatographic fingerprint for each of the samples analysed
Wavelengths: 280 nm
305 nm

Acquity SQ Detector conditions
Capillary (kV): 2.00
Source Temp (°C): 140
Desolvation Temp (°C): 420
Desolvation Gas (L/Hr): 950
Cone Gas Flow (L/Hr): 50

Two separate methods were developed for the MS conditions:
- Full scan MS (see table 2)
- MRM transitions for the targeted analysis of polyphenolic compounds

Table 2. Full scan MS conditions

Retention window (mins):	0.00 - 25.00
Scan mass range:	50 - 550
Function 1:	ES+
Function 2:	ES-

RESULTS

Current methods analysing polyphenols in fruit juice require long run-times that often are greater than 60 minutes per sample. The aim of this experiment was to transfer an existing HPLC method requiring 100 minutes per sample, to the Acquity UPLC system to improve productivity in the lab (see Figure 1).

Various fruit juices were chosen for the analysis of polyphenolic content: apple, pear, peach, grape, orange and tangerine. Eleven compounds were monitored and quantified during the analysis for confirmation of their presence or absence in the different juices. Some of these compounds were chosen as they reflect the quality of the beverage and others were selected as they are indicators of authenticity and adulteration.

Using the Acquity UPLC there are two major improvements that can be seen visually here with the chromatography:

1. **Speed:** Helps increase lab productivity - more samples analysed per instrument
2. **Resolution:** Reduces interferences from co-eluting compounds when using UV for identification

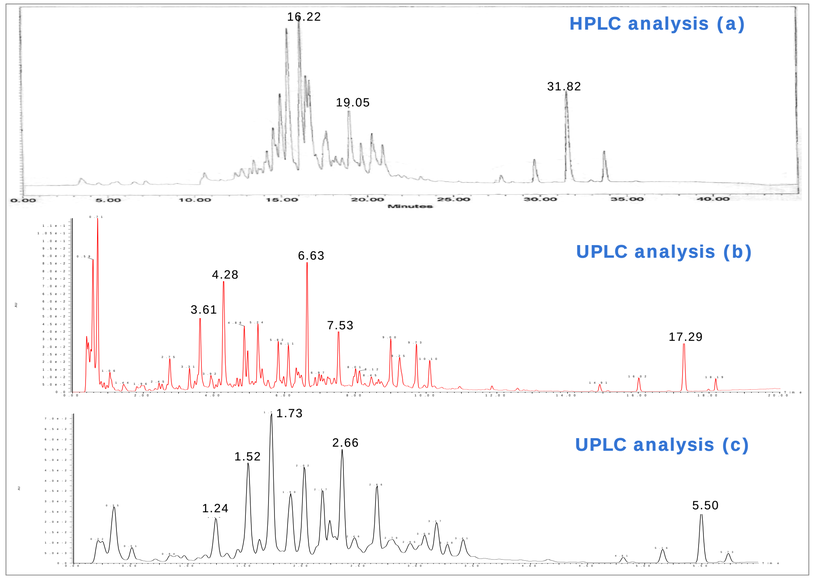

Figure 1. Analysis of the fruit beverages (tangerine sample shown here) - comparing the chromatographic differences using HPLC (a), Acquity UPLC (b) technology and UPLC-SQD (c)

DISCUSSION

During the development of this method two detectors were used for the method:-

- **UV** (most common detector for HPLC analysis of fruit juices)
- **MS** (using the mass information for confirmatory analysis)

UV Analysis
The Acquity UPLC system, in combination with 1.7um particle size columns, was used to achieve increased resolution (seen in figure 1b) and rapid run-times – the resolution of the UPLC peaks has increased compared with HPLC and increased separation can be seen. In addition to this the **100 minute** run has been reduced to less than **25 minutes** using UV.

MS Analysis
Reducing runtimes even further...
It was found that MS has many potential advantages for the analysis of fruit juices. With the addition of the Acquity SQD the speed of analysis could be reduced from: **25 to 10 minutes**—further increasing the labs efficiency (see figure 1c)

Confirming the presence of known compounds and obtaining data for unknown compounds...
Furthermore, when MS analysis was performed in full scan mode, the mass spectral information provided data to:-

- Help identify unknown compounds present in the juices (possible adulteration issues)
- Support routine analysis for new juice flavors (investigative analysis and confirming authenticity)

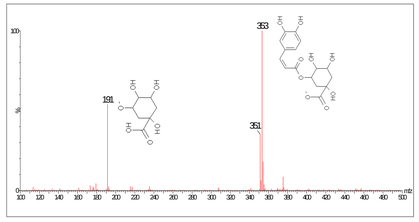

Figure 2. Confirmatory MS analysis of chlorogenic acid

CONCLUSION

The following poster has illustrated several points addressing common issues for a QC laboratory

Advantages of the Acquity UPLC

- **The implementation of UPLC into a QC laboratory is easy: here it has been shown that a routine HPLC method has been converted to the UPLC platform.**
- **By transferring from HPLC to UPLC it is possible to not only achieve excellent analytical results, such as improved resolution but it also helps the laboratory to be more efficient by reducing the bottleneck of this analysis, and also reduces operating costs.**

Advantages of the Acquity SQ Detector

- **By employing the SQ mass spectrometer with the Acquity UPLC it is possible to obtain more information.**
- **For the analysis of QC samples from a routine perspective the SQD provides additional security when quantifying known compounds.**
- **It is useful for investigative analysis: by taking advantage of the mass spectral information able to recognise any non-conforming issues such as adulteration, that may occur in the sample.**

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