AUTOMATING PREPARATION OF MATRIX-MATCHED CALIBRANTS

Adabelle ONG[1,2], Li Yan CHAN[1,2], Simon HIRD[2]
International Food and Water Research Centre[1], Waters Corporation[2]
adabelle_ong@waters.com

INTERNATIONAL FOOD & WATER RESEARCH CENTRE

Waters
THE SCIENCE OF WHAT'S POSSIBLE.™

INTRODUCTION

Preparation of standard solutions is an essential part of any quantitative testing that needs to be accurate and precise. However, this task is time-consuming, repetitive and tedious and is susceptible to human error, which can cause significant impact on the quality of the results. Automating this process would therefore minimize error, as well as reducing risk of injury (repetitive strain injury from pipetting) and allow the lab analyst to be deployed for other tasks.

Herein, we present the conventional manual pipetting and two different approaches to automate the preparation of a set of matrix -matched calibrants for pesticide residue analysis; the Andrew+ pipetting robot and the Auto-Addition function available on the ACQUITY UPLC Sample Manager.

Overall, the two automation processes greatly reduced the pipetting hours and human errors, while achieving accuracy and precision, thus maximizing productivity.

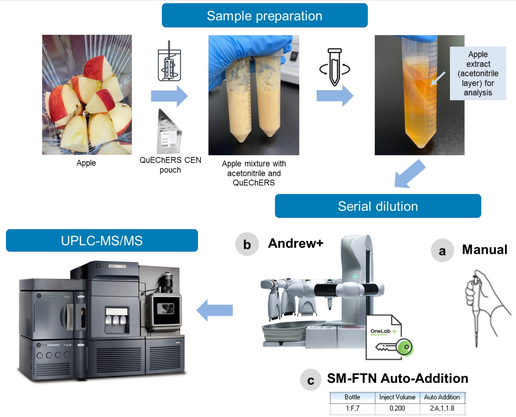


Figure 1. An illustration of the workflow — sample preparation, serial dilution by (a) manual pipetting and (b) automated pipetting and UPLC-MS/MS analysis with (c) SM-FTN auto-addition function.

METHODS

Automating preparation — Andrew+ pipetting robot

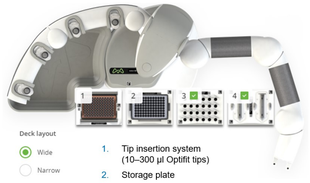


Figure 2. Andrew+ pipetting robot deck layout for sample preparation of matrix-matched calibrants using Andrew+ pipettes and domino blocks.

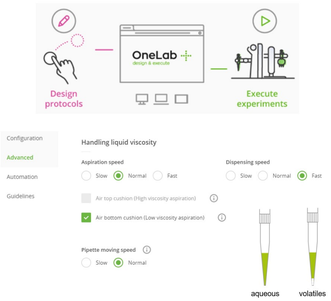
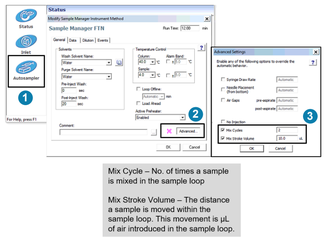


Figure 3. OneLab software allows user to trace all steps from experimental design to execution. Customized settings for different experimental needs, e.g. aqueous and volatiles require different aspiration speed.

Automating preparation — SM-FTN Auto-Addition



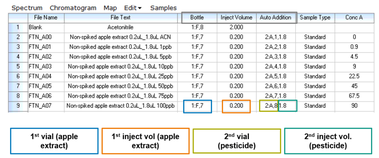


Figure 4. Automating preparation using auto-addition feature is available on ACQUITY UPLC sample manager. The functionality of the auto-addition successfully mixed multiple aliquots from different vials inside the autosampler needle to create standard solutions prior to injection.

RESULTS AND DISCUSSION

Generation of calibration curve — Andrew+ pipetting robot vs. Manual pipetting

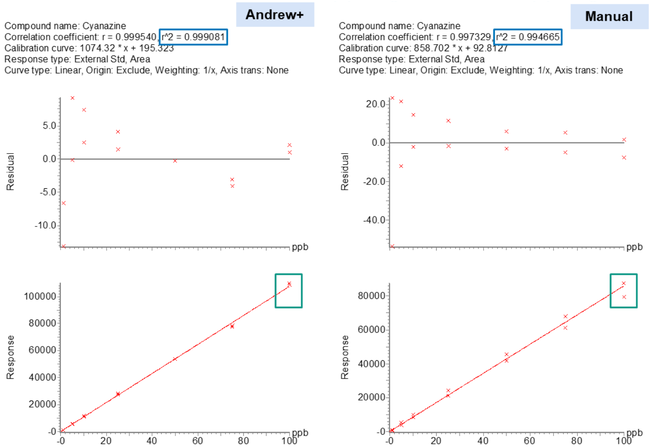


Figure 5. The calibration curve of cynazine compound by automating preparation using Andrew+ pipetting robot vs. Manual pipetting show excellent linear correlation coefficient r^2 of 0.999 and 0.995 respectively. This reflects accuracy, consistency and reproducibility across both pipetting methods. The Andrew+ pipetting completed more than four times faster than manual pipetting done by a typical lab analyst and reduces potential risk of human error and smaller residual range.

Effect of Direct injection and Auto-Addition in acetonitrile injection solvent

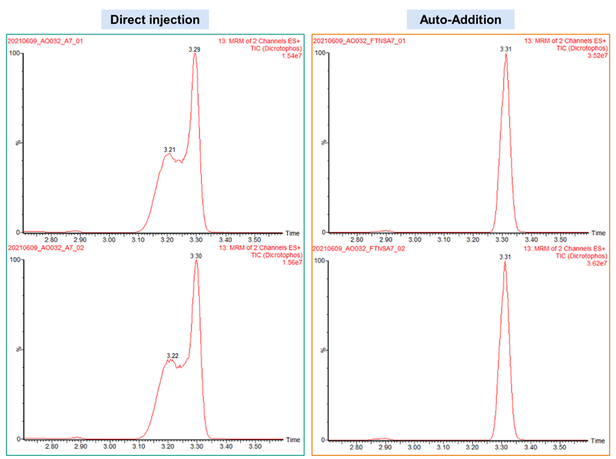


Figure 6. Representative UPLC-MS/MS chromatograms of one of the pesticide compounds, dicrotophos in 100% acetonitrile using direct injection vs. auto-addition functionality . The auto-addition feature has an additional advantage by mixing with the initial mobile phase to improve the peak shape.

BENEFITS

Andrew+	Manual
• Fully automated process which can be completed in 13 min 50 secs	• Manual process which required 1 hour 1 min 16 secs
• Increase walk-away time with automated workflow	• Tedious and repetitive task
• Easy to use with minimal training required	• Higher risk of human error especially when handling large volume of samples
• Reproducible and consistent pipetting results	
• Accurate and precise quantification performance	
• OneLab software to guide user and automate method transferability	
• Reduces the need for repetitive pipetting which can lead to repetitive strain injury	
• Minimises exposure to hazardous chemicals in some experimental procedures	

Productivity

Reproducibility

Promoting health

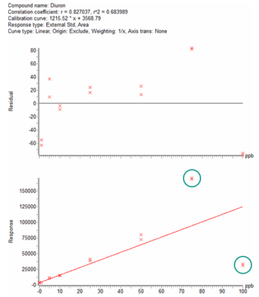


Figure 7. The use of automating preparation, Andrew+ pipetting robot helps to increase productivity, reproducibility and reduces potential risk of error encountered in manual preparation.

CONCLUSION

- **The automated method developed on Andrew+ has demonstrated comparable results to manual pipetting.**
- **Andrew+ results delivered higher reproducibility in most compounds.**
- **The use of Andrew+ pipetting robot has significantly reduced the 'hands-on' time and risk of user error.**
- **Utilization of SM-FTN auto-addition feature to prepare standard solutions further improved consistency and reproducibility with the help of mixing prior to injection.**

Andrew Alliance
A WATERS COMPANY

Andrew
the pipetting robot

References

1. D Shah, J Wood, G Fujimoto, E McCall, S Hird, and P Hancock. Multiresidue Method for the Quantification of Pesticides in Fruits, Vegetables, Cereals and Black Tea using UPLC-MS/MS. Waters application note no., 720006886en. February, 2021.
2. M Trudeau and N Skinner. Demonstration of LC-MS Nitrosamine Impurity Quantification Performance using Automated Sample Preparation with the Andrew+ Pipetting Robot. Waters application note no., 720007134en. January 2021.
3. D Shah, E McCall, and G Cleland. Single LC-MS/MS Method for Confirmation and Quantification of Over 400 Pesticides in a Complex Matrix Without Compromising Data Quality. Waters application note no., 720005559en. January, 2016.

TO DOWNLOAD A COPY OF THIS POSTER, VISIT WWW.WATERS.COM/POSTERS