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Bioanalytical Method Development with UNIFI: Promoted Parameters

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APPLICATION BENEFITS

The promotable parameter function within the Waters UNIFI Scientific Information System facilitates the rapid acquisition of the data required to select the optimal LC and MS conditions for a bioanalytical assay.

WATERS SOLUTIONS

Regulated Bioanalysis System Solution

UNIFI™ Scientific Information System

KEY WORDS

Promoted parameters, clopidogrel

INTRODUCTION

The development of bioanalytical methodologies requires the evaluation of multiple chromatographic, sample preparation, and mass spectrometry parameters and conditions. This often requires multiple iterations of changing experimental conditions, reviewing results, and performing follow-up experiments.

These tasks require a significant amount of manual input and are typically performed by expert or experienced scientists. The use of a simple template-driven process allows the rapid, simple evaluation of all LC and MS parameters required to select the optimal method parameters. Previous LC/MS data systems did not have the flexibility to allow all of these parameters to be varied and tested in a simple straightforward manner.

Figure 1. UNIFI Scientific Information System

The UNIFI Scientific Information System allows for the evaluation of many acquisition variables via the promotable parameters function. This approach allows the scientist to promote the experimental variable (e.g., capillary voltage) to be evaluated within the acquisition run list. The user can then vary the value of the parameter to be changed from injection to injection.

RESULTS AND DISCUSSION

The UNIFI Scientific Information System is equipped with a highly flexible interface, which allows the scientist to select specific parameters that need to be investigated. Once created, the sample list can be saved as a template for future use.

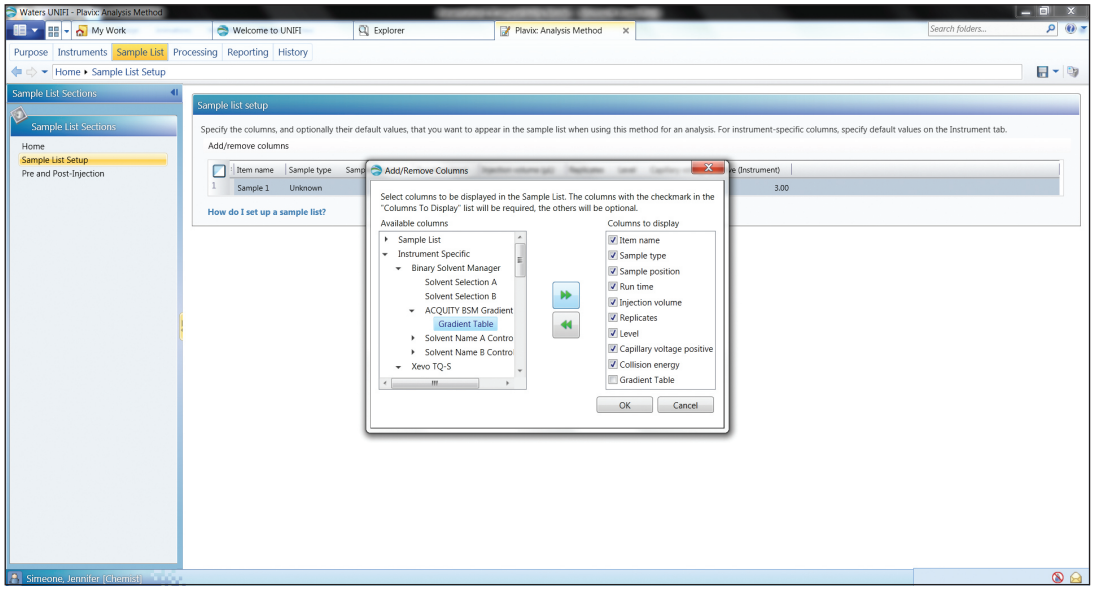

Figure 2. Creation of acquisition sample list with promotable parameters.

The ability to select and vary multiple experimental method parameters, column chemistry, mobile phases/ modifiers, capillary voltage, collision energy etc, in one simple data acquisition allows the scientist to acquire all the necessary data to identify the best LCMS conditions quickly and efficiently.

The use of this approach is demonstrated in Figure 3 for the evaluation of the effect of changing the column temperature on analyte selectivity and sensitivity for the quantification of clopidogrel in extracted human plasma.

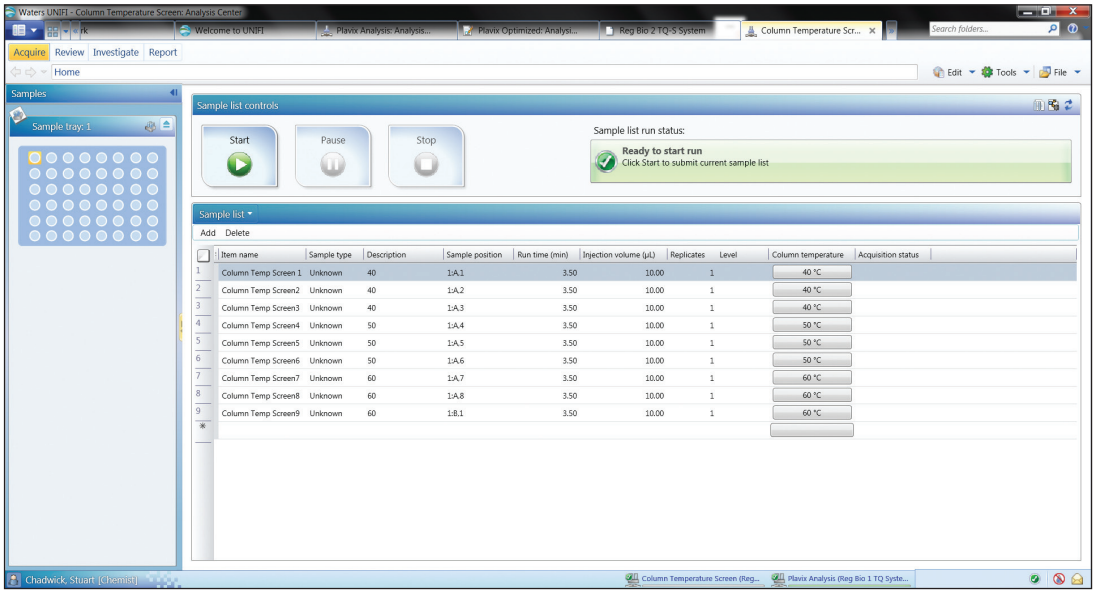

Figure 3. Evaluating the effect of a change in column temperature using UNIFI

CONCLUSION

The promotable parameter function within the Waters UNIFI Scientific Information System facilitates the rapid acquisition of the data required to select the optimal LC and MS conditions for a bioanalytical assay. The benefits to the scientist are:

- Parameters to be varied can be selected and saved in a template for future use
- Improved productivity
- Greater number of parameters can be evaluated for optimal method selection
- Reduced need for expert user

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February 2012 720004286en AG-PDF

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