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Bioanalytical Method Development with UNIFI: Compound Optimization for MRM Analysis

Waters Corporation

This is an Application Brief and does not contain a detailed Experimental section.

Abstract

The compound optimization functionality within the UNIFI Scientific Information System, part of the Regulated Bioanalysis System Solution, facilitates the fast, simple development of an MRM method for one or more compounds. The results generated can then be stored within the scientific library in the UNIFI System, allowing simple method generation and sharing of information between scientists.

Benefits

The compound optimization within the Waters UNIFI Scientific Information System delivers a fast, simple, consistent, and automated solution for the development of mass spectrometry multiple reaction monitoring (MRM) methodologies for bioanalytical studies.

Introduction

Successful bioanalysis relies on the development and validation of a reliable, robust, reproducible LC-MS methodology. A key component of this methodology is the mass spectrometry MRM method. Evaluating and developing this MRM method can be a long, exhaustive process requiring the evaluation of multiple parameters, such as: precursor and product ion combination, collision energy, temperatures and gas flows.

This process is not only time-consuming but often requires an experienced scientist to extract the optimal conditions. Additionally, the conditions once developed are typically confined to a study file and/or SOP and are not readily searchable by other scientists within the organization.

Results and Discussion

The UNIFI Scientific Information System has been designed to allow the scientist to manage, execute and store their analysis in a secure and compliant environment.

Figure 1 . UNIFI Scientific Information System

Once initiated, the laboratory data is contained and accessed within the UNIFI System via the “My Work” domain. Developing a new MRM method is performed via the “Compound Optimization” function (highlighted in red in Figure 2). The scientist is then able to input the ranges for each of the individual

parameters to be explored. This is controlled via an automated sequence of option boxes.

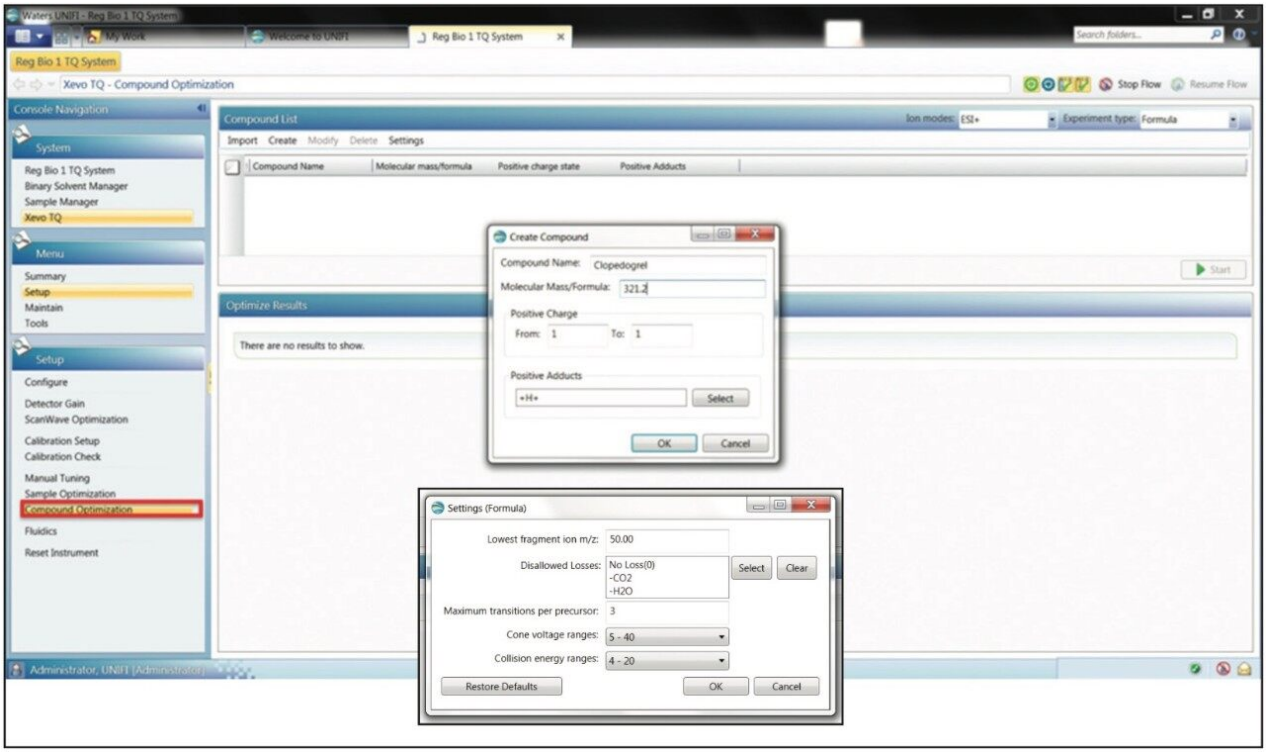

Figure 2. Developing an MRM method, top, and inputting parameters, bottom.

This functionality is illustrated in Figure 3 where capillary voltage, cone voltage range, collision energy range, and infusion sample location are selected. Undesired fragments such as the loss of water or CO_2 can be defined via a dropdown menu, ensuring a specific assay is developed free from interferences.

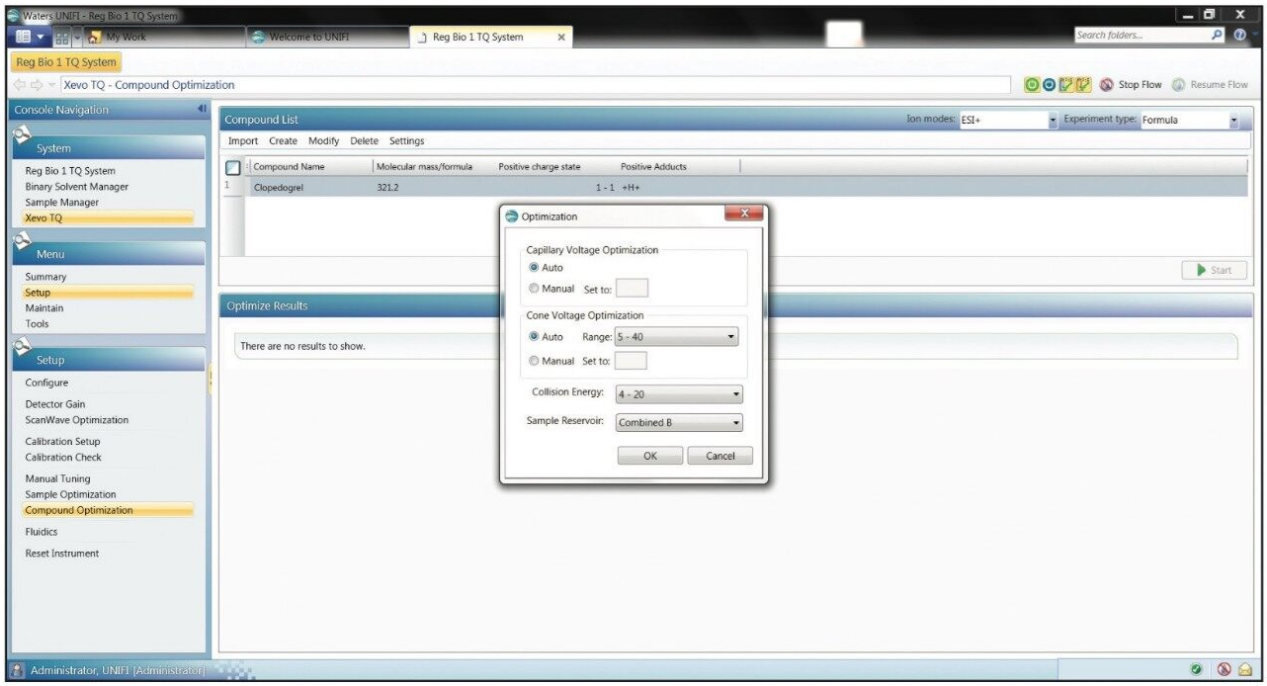

Figure 3. Selecting the mass spectrometer's conditions.

Once the evaluation ranges for all of the MS parameters have been defined, the system automatically infuses the sample and acquires the necessary data. At the end of the acquisition, the data is saved and then displayed as a report to the scientist as shown in Figure 4.

Compound Name	Precursor	Precursor Mass	Product Mass	Ion Mode	Capillary Voltage	Cone Voltage	Collision Energy	Intensity
Clopidogrel	[M+H]+	322.10	183.89	ESI+	0.50	23.00	20.00	6019263.4637428
Clopidogrel	[M+H]+	322.10	211.88	ESI+	0.50	23.00	18.00	14574179.383543

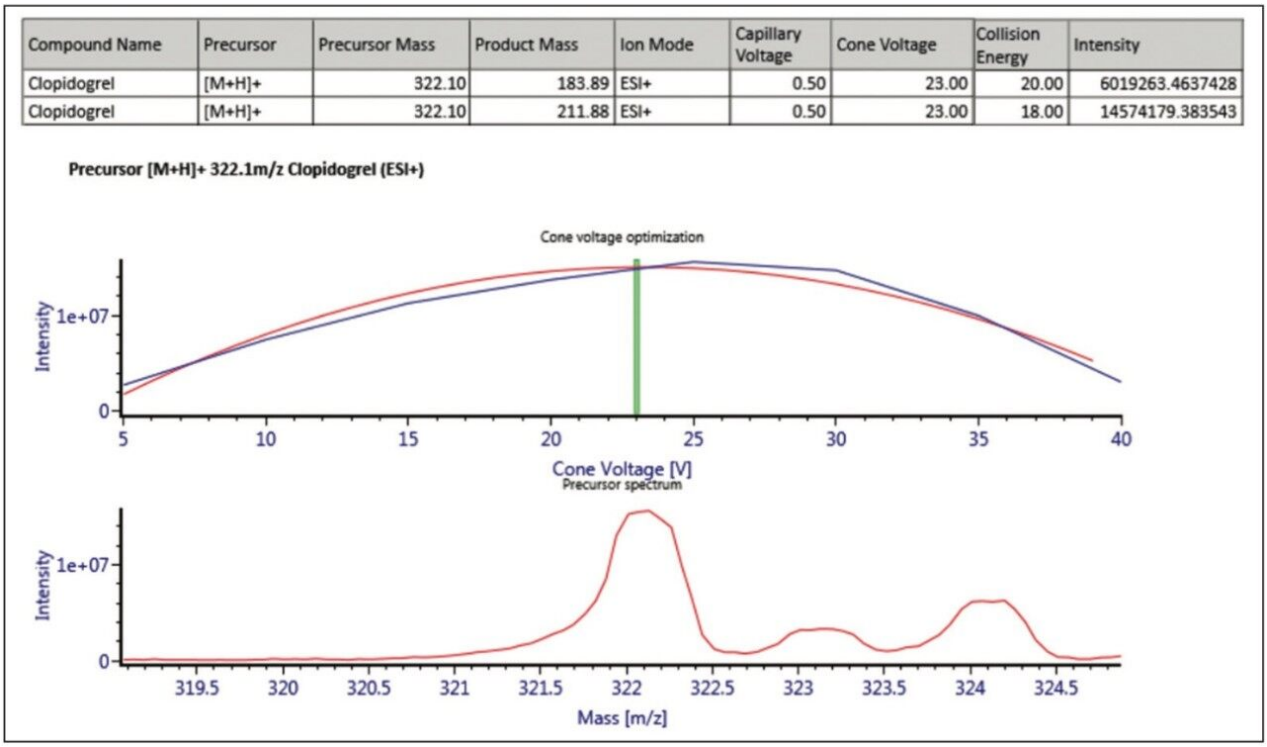

Figure 4. Saving acquisition data.

The resulting MRM transitions, containing the optimized voltages and collision energies, are presented to the scientist in a tabular form. The scientist can then select the transitions best suited for the analysis at hand. These conditions are then exported to the “scientific library” within the UNIFI System for incorporation into the LC-MS method.

The UNIFI Scientific Information System is designed to operate in a workgroup or enterprise environment, with many users connected to and sharing a common central data server. Saving the optimized MS conditions in the scientific library allows them to be searched by any other scientist with access to the system. This functionality allows simple, fast searching of compounds or compound classes, promoting information sharing and productivity, while maintaining a streamlined operation.

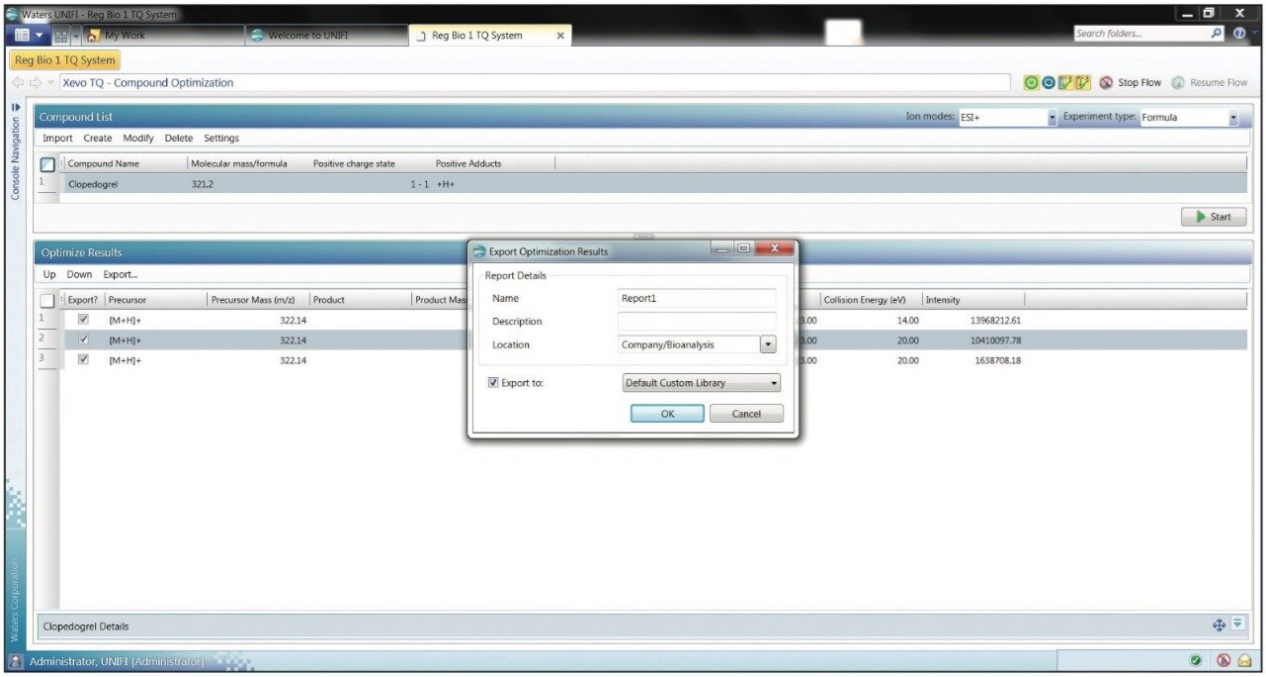

Figure 5. Exporting optimization results.

Conclusion

The compound optimization functionality within the UNIFI Scientific Information System, part of the Regulated Bioanalysis System Solution, facilitates the fast, simple development of an MRM method for one or more compounds. The results generated can then be stored within the scientific library in the UNIFI System, allowing simple method generation and sharing of information between scientists. This functionality:

- Improves productivity
- Ensures consistency of operation
- Ensures the most selective and specific parameters are chosen
- Promotes efficient sharing of data
- Reduces the need for expert operation

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UNIFI Scientific Information System <https://www.waters.com/134801648>

Regulated Bioanalysis Platform Solution with UNIFI <https://www.waters.com/134613325>

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