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WHITE PAPER 72749

Using the Thermo Scientific Vanquish UHPLC or UltiMate 3000 SD HPLC system with the Waters Empower 3 chromatography data system (CDS)

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### **Keywords**

Vanquish UHPLC instruments, UltiMate 3000 HPLC instruments, Thermo Scientific SII for Empower software

### Goal

This paper describes the operation of a Thermo Scientific<sup>™</sup> Vanquish<sup>™</sup> UHPLC system and a Thermo Scientific<sup>™</sup> UltiMate<sup>™</sup> 3000 HPLC system under Waters<sup>™</sup> Empower<sup>™</sup> 3 software control. Screen shots, technical information and considerations on qualifying a Thermo Scientific-branded chromatography system under Empower 3 software demonstrate the user experience and provide valuable insights for system administrators and quality managers. In addition, the paper highlights selected strengths of the Vanquish UHPLC platform controlled by the Thermo Scientific Standard Instrument Integration (SII) driver under Empower 3 software.



### Introduction

The pharmaceutical industry, whether producing large or small therapeutically active entities, has asked HPLC manufacturers for many years to provide more unified software for system control and data processing. The impact on training efforts, logistics (networking), data exchange and data integrity is significant for the industry.

Thermo Scientific<sup>™</sup> Chromeleon<sup>™</sup> 7.2 CDS is the recommended software for control of Thermo Scientific UHPLC and HPLC instruments as it offers unique, smart features that deliver maximum ease of use, reliability and performance. However, in the modern laboratory it is expected that these instruments can be incorporated and operated within other vendors' CDS systems. This white paper describes how one of the leading UHPLC and HPLC platforms in the market can be operated and controlled by Waters Empower 3 software. From a user-experience perspective and from a supporting IT perspective, very few changes are required. After the SII driver for Empower 3 software is installed on all Waters<sup>®</sup> LAC/E<sup>32™</sup> Acquisition Server boxes connected to a Thermo Scientific LC as well as on, for example, a Citrix<sup>®</sup>-type light client server, the Empower 3 software environment continues to administer all aspects of the CDS. Only after instrument methods are written and the startup/shutdown of the Vanguish UHPLC system or the UltiMate 3000 SD HPLC system is performed do the uniquely integrated system controls appear with native real-time control panels or instrument method wizards.

The SII driver does not offer a diluted version of system commands or control options. On the contrary, the driver offers the complete set of commands as they are present under native Chromeleon CDS control. For the user this means that tools and the advanced features applied for two-dimensional LC, tandem operation or simply preparing the next sample during an ongoing run, can be implemented to increase productivity and receive more data with fewer injections. In addition, the driver also offers integration of Thermo Scientific branded ion chromatography systems. Installation and operational qualification is optional and provided by trained Thermo Fisher Scientific ULS engineers under Empower 3 software control to ensure complete data integrity.

### **Application example**

The use of HPLC equipment from multiple manufacturers is a common situation in pharmaceutical laboratories. A disadvantage of this is that it often involves the use of different chromatography data and control software. Therefore, users and lab managers have frequently asked instrument vendors to enable the integration of their hardware into another vendor's software system. This can significantly reduce the maintenance efforts for the laboratory's CDS and reduce training efforts.

Here, we use a Thermo Scientific<sup>™</sup> Vanquish<sup>™</sup> Horizon UHPLC system controlled under Empower 3 software with the applicable USP method for ibuprofen.<sup>1</sup> From the original USP method for determination of the main active ingredient in tablets, we developed a fast UHPLC method that is a perfect example of the Empower 3 software integration and how to boost the assay's productivity and potentially accelerate batch release testing. For more details on the application refer to Reference 2.



Vanquish UHPLC system



UltiMate 3000 HPLC system

### Step 1: Configuring instruments

After the full installation of the Empower 3 software and SII driver for Empower, the Vanquish Horizon UHPLC instrument was configured using the system setup in SII for Empower software. Next, the system was simply added in the Empower 3 Configuration (Figure 1). Thus, a flawless integration of the Vanquish instrument into Empower 3 software was obtained.



The "Configure the System" section in Empower 3 software is very helpful for setting up basic functionalities like Projects, Systems, User Types and Privileges, as well as Plate Types of the

Vanquish and UltiMate autosamplers. If you need assistance in configuring plate types, go to the Help function in SII for Empower software and search for "plate types". You can also import predefined Thermo Scientific and Dionex plate formats as .txt files, which are provided with the SII driver installation DVD. A detailed description of defining and configuring plates of all available types of autosamplers will be displayed.



System setup in SII for Empower software

Empower on Local a	s System/Administrator	
00		Empower®3
0	Configure the System Perform administrative tasks in configu	ration manager.
•	Run Samples Select Project and Chromatographic sy	stems to acquire data.
0	Browse Projects View and select Project to open.	
🔁 Logout		🔁 Login new user
Empower	3 software	



Empower 3 software configuration

Figure 1. Instrument configuration

## Step 2: Controlling the instrument in Empower 3 software

After connecting all the modules, it is very easy to control the pump, autosampler, oven and detector and prepare them for the upcoming measurements. In the Empower software instrument control section, a compact panel set is provided delivering key system controls directly to the user. This includes purging solvent lines, setting flow rates and column temperature, as well as switching on and off the detector lamp(s). In addition, the SII for Empower interface can be used to access all controls and parameters for the instrument. Figure 2 shows both options.



Use the Launch Instrument View option to switch from instrument control in Empower 3 software to the SII for Empower interface for controlling the instrument.

### Step 3: Writing instrument methods

Setting up an instrument method is simple, intuitive and fast. The wizard guides you through all the modules, where you can enter the necessary information about the method (Figure 3).



Instrument control in Empower 3 software

Instrument control in SII for Empower software

Figure 2. Instrument control

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Solvents	General Settings for SamplerModule (VH-A10-A).		Sillurtan					
Name		Temperature Settings for ColumnComp (VH-C10-A).	Janayakan					
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10. Lestenhile 0.1% Famile Anid (1)								
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	Injection wash procedure parameters	Ready temp. delta: 0.50 V (10.055.00 °C)	2 VUV VIS 2 254.0 4 Off 4 Start Run Stop Run					
Pressure Limits Maximum Flow	Wash mode:	Equilibration time:	3 VUV_VTS_3 270.0 4 Off 4 Start Run Stop Run					
	Now/ath man	E gand and rates. I The State of the state o	4 VUV_VIS_4 300.0 4 Off 4 Start Run Stop Run					
Lower Limit: 0 🥹 (01034 bar) Ug: Infini	Wash gme: BeforeDraw (0.0	Themostatting mode: StillAir - 🗸	Sart Kun Sop Kun					
Henry Livit: 1000	Wash speed Both [10.0.	Ean speed: 5 (2) (07)						
The run hoo A for long at Town hum								
	Connected pump	Pre-Heater	In initial experiments, we recommend to acquire data with RefWavelength set to OII.					
	Fine is delivered from	Line temperature construit	Data Collection					
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	Sample puncture	Heady temp: getta: 11.00 • 9 1.00 • 9 10.05_5	Peak Width: 0.020 (0.000_10.000 min) may lead to increased noise or increased noise or					
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			Beady					

Figure 3. Program Wizard for instrument method setup

After completion, the full method can be checked for errors before starting the set of experiments (Figure 4).



Figure 4. Error checking

## Step 4: Setting up a method set and running samples

In addition to the instrument method, the method set may also contain a processing and report method (Figure 5). These can be assigned to one or more samples by choosing the name from the drop-down menu. The run time entered in the sample set table must be the same as in the instrument method used.



Naming the method set the same as instrument method helps later in the assignment of the instrument method to each injection.



**Method Set** 

					-	Sar	nple Set Method: Ibu	calibration speed up					
E	rack/vial	lnj Vol (uL)	# of Injs	Label	SampleName	Level	Function	Method Set / Report or Export Method	Label Reference	Processing	Run Time (Minutes)	Data Start (Minutes)	Next I Dela (Minut)
1	R:B,6	0.1	1		Blank FM		Inject Samples	IBU_VAL_Speed_up		Normal	1.00	0.00	0
2	R:B,1	0.1	1		ibu 1 ngihi.		Inject Samples	IBU_VAL_Speed_up		Normal	1.00	0.00	0
3	R:8,2	0.1	1		Ibu 2.5 mg/mL		Inject Samples	BU_VAL_Speed_up		Normal	1.00	0.00	0
4	R:8,3	0.1	1		Ibu 5 nginL		Inject Samples	BU_VAL_Speed_up		Normal	1.00	0.00	0
5	R:8,4	0.1	1		Ibu 7.5 mg/mL		Inject Samples	BU_VAL_Speed_up		Normal	1.00	0.00	0
6	R:8,5	0.1	1		Ibu 10 mg/mL	1	Inject Samples	IBU_VAL_Speed_up		Normal	1.00	0.00	0
7	R:B,6	0.1	1		Blank FM		Inject Samples	BU_VAL_Speed_up		Normal	1.00	0.00	0
8	RA,4	0.1	1		lbu tablet 29.01.2018		Inject Samples	BU_VAL_Speed_up		Normal	1.00	0.00	0
9	RB,6	0.1	1		Blank FM		Inject Samples	BU_VAL_Speed_up		Normal	1.00	0.00	0
10	R:8,7	0.1	1		Ibu Recovery Singlini.		Inject Samples	IBU_VAL_Speed_up		Normal	1.00	0.00	0
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Sample Set



Online Plot

Figure 5. Method Editor

### Step 5: Data processing

The data processing, including quantitative data evaluation, can be done by applying an appropriate processing method. For this purpose, calibration samples must be assigned and a calibration curve compiled. The quantitative amounts of each sample can be directly calculated within the software and all results can be saved in a complete results file, which makes it very convenient to reload and review data (Figure 6).



Complete data processing takes place inside Empower software, which allows you to use all functionalities as you would normally, for example, overlay

of chromatograms or other channels like pressure traces. The Empower user experience does not change for any data processing aspect.



Figure 6. Data processing

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### Conclusions

- Flawless integration of Vanquish and UltiMate SD instruments into Empower 3 software without loss of functionalities
- Instrument control, data acquisition and data processing performed completely under Empower 3 CDS
- Reduced network logistics and training efforts

#### References

- 1. United States Pharmacopeia and National Formulary USP 40-NF 35; The United States Pharmacopeial Convention, Inc: Rockville MD; 2017. Ibuprofen; p 4555-4559.
- Grosse, S.; De Pra, M; Steiner F. Fast methods for the determination of ibuprofen in drug products; Thermo Scientific Application Note 72709; June 2018. https://assets. thermofisher.com/TFS-Assets/CMD/Application-Notes/an-72709-Ic-ibuprofen-drugproducts-an72709-en.pdf

#### Additional resources

- a. Thermo Scientific Application Note 21680: A rapid ibuprofen USP assay method https://assets.thermofisher.com/TFS-Assets/CMD/Application-Notes/AN-21680-LC-Ibuprofen-USP-Monograph-Modernization-AN21680-EN.pdf
- b. Flyer: Thermo Scientific HPLC and UHPLC systems controlled by Empower 3
- c. Videos: User experience using Thermo Scientific HPLC and UHPLC systems with SII on Empower 3 CDS
- d. SII for Empower online help (provided with the SII driver installation DVD)

### Learn more at thermofisher.com/liquidchromatography

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