

# Cliquid® ChemoView™ 3.0 Software

Simple automated analysis, from sample to report

## KEY FEATURES

- Secure user login that links the identity of an operator to the ability to run specific tasks
- Customizable, simple 4-step workflow
- One click process for loading LC/MS/MS methods
- Compatible with iMethod™ Tests
- Create new or customize methods
- Pack/unpack feature to share acquisition methods
- Quickly screen for compounds in large data sets
- Set predetermined limits for each analyte
- Highlight results outside of limits specified
- Specify report templates by method
- Batch process results across sample types
- Full control of leading HPLC systems
- Easy to use Windows based reporting tool
- Simplified data analysis tools
- Full compatibility with Analyst® Software version 1.5.1



## INTRODUCTION

Tandem mass spectrometry has become the technique of choice for both screening and confirmation of metabolic disorders due to the simplification of sample preparation, sensitivity and selectivity, the speed of analysis, and the ability to measure more than one analyte across different compound classes simultaneously. These advantages result in a lower cost per sample analysis than traditional techniques.

Cliquid® ChemoView™ 3.0 Software from AB SCIEX is now accessible through the Cliquid 3.0 software via the addition of a Cliquid® ChemoView 3.0 license. This simplifies the operation of LC/MS/MS to a customizable, simple 4-step workflow while harnessing the data processing power of the ChemoView™ 2.0.1 Software. Cliquid®

ChemoView™ 3.0 Software is designed for easy acquisition and data processing to aid researchers who want to quickly screen a series of compounds in a large set of flow injection triple quadrupole mass spectrometry (FI/MS/MS) data. Application areas include: research into inborn errors of metabolism (IEM), metabolic studies, lipid and endocrine studies and acylcarnitine profiling. Many classes of analytes can be added to the list of compounds. The most common are amino acids (AA), acylcarnitines (AC), sugars, fatty acids, peptides and proteins. The tandem mass spectrometry scanning methods available are Precursor Ion Scan (PS), Neutral Loss Scan (NL) and Multiple Reaction Monitoring (MRM).

Built with an intuitive point and click interface, Cliquant® ChemoView™ 3.0 Software provides the ability to use preconfigured LC/MS/MS iMethod™ Tests and reporting tools. Cliquant® ChemoView™ 3.0 Software also provides the flexibility to create and add new tests specific to laboratories' needs and to manage the tremendous amount of data generated in high throughput screening applications.

### SECURE LOGIN AND HOME PAGE

Upon launch, a password is required to enter the software. Once logged in, the graphical user interface of Cliquant® ChemoView™ 3.0 Software is displayed (Figure 1). The content of the page is based upon the user rights set up in the system. Some users will only be able to run samples and generate reports while others can set up new tests and report styles.



Figure 1. Secure user login links the identity of an operator to the ability to run specific tasks.

### EASY-TO-USE

The panels in Figure 2 on the left hand side of the screen denote the 4-step workflow in performing the analysis: choosing the test to be run; building the sample list; choosing the type of report and report delivery options and submitting the samples for analysis. The instrument panel at the bottom of the screen indicates the status of the HPLC and MS/MS systems. Green presents a successfully acquiring system while yellow indicates that all components are in standby or warming up. In the case of any hardware error the status of the corresponding component will change to red.

#### STEP 1: CHOOSING THE TEST

The first step of the 4-step workflow is to choose the required test, which is done by clicking on the appropriate radial button. All of the HPLC and MS/MS parameters are automatically loaded. A click on the icon next to the test will provide method details associated with each test.

#### STEP 2: BUILDING A SAMPLE LIST

Cliquant® ChemoView™ 3.0 Software provides an easy way to create sample lists for plates to be analyzed. Simply enter the sample name,

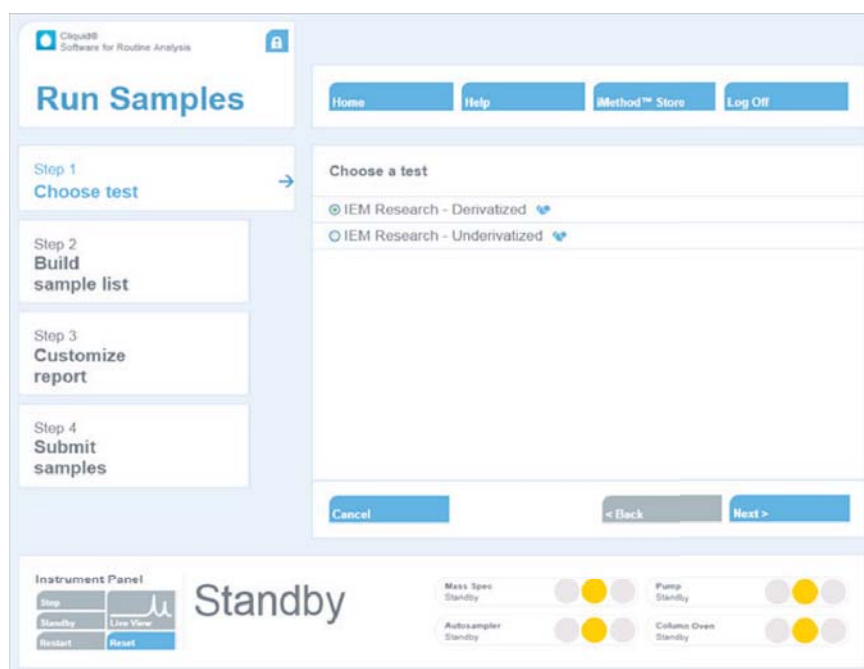


Figure 2. Cliquant® ChemoView™ 3.0 Software workflow.

sample position and sample type. Alternatively, Cliquid® ChemoView™ 3.0 Software sample lists can be automatically loaded from properly formatted work lists created in Excel or other compatible programs. Cliquid® ChemoView™ 3.0 Software allows real time sample monitoring and data viewing as the samples are processed. Sample lists are set up as batches to increase the speed and efficiency of reporting.

### STEP 3: SELECTING THE REPORT FORMAT

Various preconfigured and customizable report styles are available. Additionally, delivery options can be specified which include saving the report as a Word document or pdf file, printing the report or automatically emailing the report once completed. The system can also generate a report after each run or provide a summary report for the entire sample batch upon completion (Figure 3).

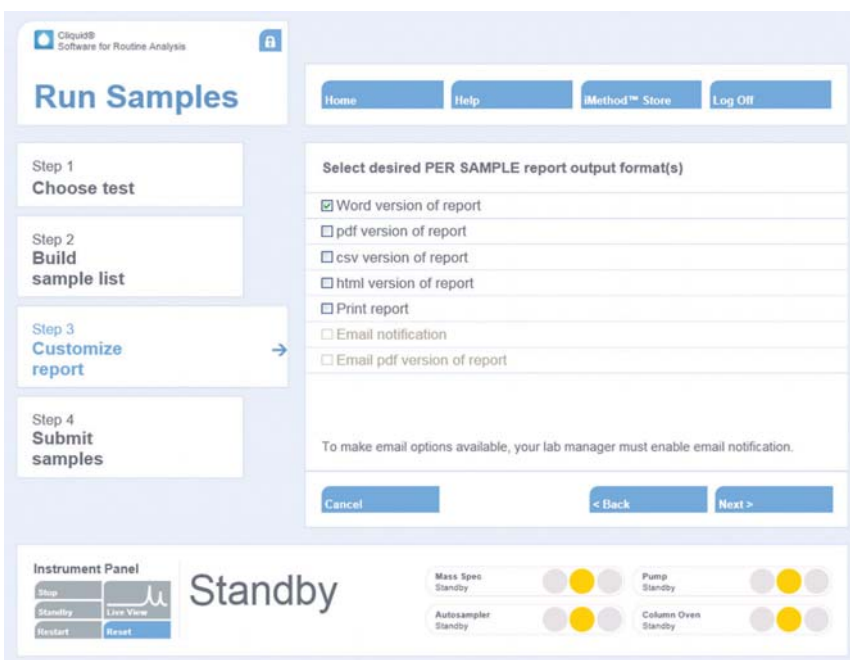


Figure 3. Customize your report.

### STEP 4: SUBMITTING THE SAMPLE

The last step is to submit the sample information to the LC/MS/MS system in order to start the analysis. Before proceeding with the analysis, a dialogue box appears in the middle of the screen to confirm the test selected, and that the appropriate solutions are present. After submission, a sample and report list will be displayed to monitor the progress of acquisition and report generation. Green check-mark status symbols indicate if a sample is finished (Figure 4). During acquisition, the order of waiting samples can be changed including moving an emergency sample to the very top of the sample list. A live view of the chromatogram currently being obtained can be accessed by clicking on the live view button at the bottom left of the screen (Figure 5). Once the analysis is completed reports are automatically generated. Clicking a view button at the report list will display the completed report (Figure 6). In addition to a broad range of standard reports the built-in reporting tool provides the possibility to modify existing and to implement new report styles according to specific laboratory requirements.

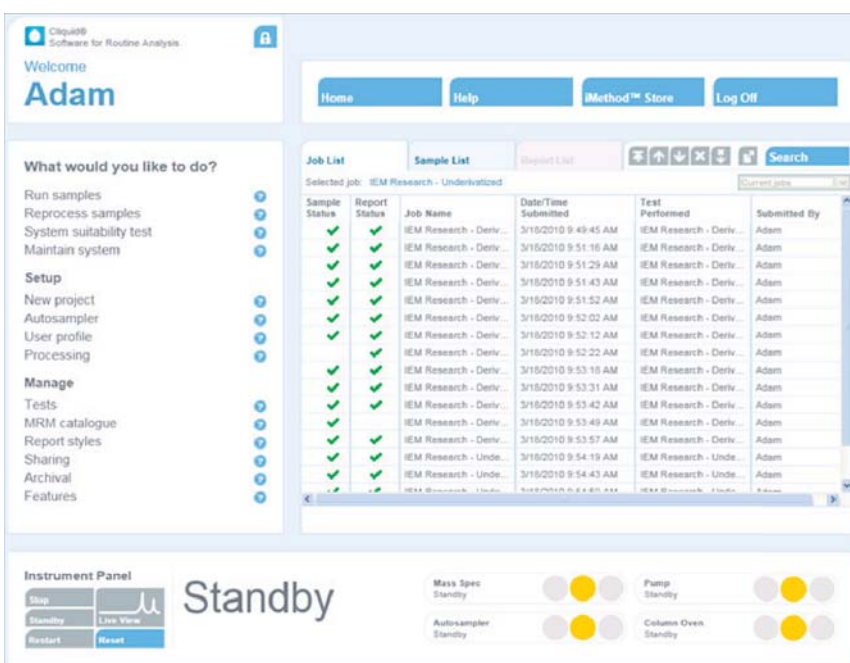


Figure 4. Sample processing status.

## SUMMARY

Cliquis® ChemoView™ 3.0 Software simplifies the use of LC/MS/MS for routine testing. It is built with an intuitive point-and-click interface, four step workflow, and powerful data analysis tools with ChemoView™ 2.0.1 Software. ChemoView™ 2.01 Software is an excellent tool to set up data review test parameters, design tests, screen for analytes or create distinct sample types, each with its own flagging limits and process data to produce reports. If the acceptance limits for the compounds have been established, the program highlights the samples that have results outside of the limits. Cliquis® ChemoView™ 3.0 Software flags any samples observed to exceed user defined thresholds and generates the requested reports or sample print outs. Several preconfigured report templates are available for immediate use or for customizing. The reports can be generated as a Word document, pdf file, Excel (csv format) or html file. Reports are printed automatically, emailed, or stored in a specified location. Cliquis® ChemoView™ 3.0 Software simplifies the process from the running of samples to the generation of results.

Cliquis® ChemoView™ 3.0 Software requires Cliquis® 3.0 and is used with Analyst® Software Version 1.5 or higher. The software can be used with any AB SCIEX QTRAP® or triple quadrupole LC/MS/MS System. Alternatively, Cliquis® ChemoView™ 3.0 Software can be purchased as part of a starter pack that includes everything your lab will need to get up and running quickly for IEM research. The IEM Research starter pack includes an API 2000™ LC/MS/MS System, an Agilent 1200 LC system, Analyst® 1.5.1 Software and both Cliquis® Software 3.0 and a Cliquis® ChemoView™ 3.0 Software license. The starter pack also includes a preconfigured iMethod™ Test for the analysis of amino acids and acylcarnitines.



Figure 5. Viewing the data chromatogram.

Test Name	Result	Units	Qualifier	LCL	UCL
FreeCN	0.194	µM	FAILED_TOO_LOW	9	60
HydroAC	3.799	µM	PASSED	0	∞
C2	0.132	µM	PASSED	0	80
C2-Glu	0.169	µM	PASSED	0	25
C3_C2	0.051	µM	PASSED	0	0.2
C2_C2Glu	0.782	µM	FAILED_TOO_LOW	1.25	100
C3	0.007	µM	FAILED_TOO_LOW	0.2	5.25
C4	0.001	µM	PASSED	0	1.4
C5-1	0.007	µM	PASSED	0	0.14
C5	0.005	µM	PASSED	0	0.5
C4-OH	0.017	µM	PASSED	0	0.75
C6	0.011	µM	PASSED	0	0.24
C5-OH	0.013	µM	PASSED	0	0.6

Figure 6. Report preview.

For more information on Cliquant®  
ChemoView™ 3.0 Software and how it can  
be used with AB SCIEX products please  
contact your local sales representative  
or visit our web site:

**[www.absciex.com/clinicalresearch](http://www.absciex.com/clinicalresearch)**.

See the product note for ChemoView™ 2.0.1  
Software for additional software functionality  
(114PB43-01).

#### **iMETHOD™ TESTS**

iMethod™ Tests reduce method development  
and deployment time for a range of popular  
applications, and provide instant access  
to lab-proven methods through Cliquant®  
Software. To acquire and process data  
using this software, you must have the  
Analyst® Software version 1.5 or higher,  
Office 2003 or 2007 (Word and Excel),  
and the ChemoView™ Software 2.0.1  
standalone application installed on the  
acquisition computer.

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