Software Status Bulletin
6400 Series Triple Quadrupole LC/MS Bundle
MassHunter WorkStation Acquisition Software rev. B.06.00

Revision Log:

Revision Date	Reason For Update
16 November 2012	**Initial revision**
21 November 2012	**Modified content**

1. Overview

The purpose of this document is to list known problems in the software and any known workarounds or recovery paths.

2. Known Problem Summary

The following is a summary of the known problems in the software. This is not an exhaustive list, but is a list of the problems a customer is most likely to encounter. This list cross-references items in our Defect tracking database.

2.1 Tuning

Team Track #	
180007	Clicking on the Tune file Browse button, brings up worklist select instead
183592	Method pane type mismatch exception after switching back from Tune context and trying to load a method
195805	Diverter valve error at end of autotune

2.2 Acquisition

Team Track #	Title
178134	Time segments not updating on DMRM run with Waste time segments
185743	"Script Help" tab in scripts don't have required information.
191617	6490 tune file loaded on 6460 instrument will not allow parameters to be downloaded to instrument
193725	Run parameter error fault in MS.
194801	Run acquisition with wrong ion source in method got software into hung state
196037	Slightly different peptides with same transitions and different RTs lead to only first peptide being collected
196471	CE defined in Acq Method is not acquired when you look at data file
196476	iFunnel parameters will not be set from tune file values in Offline Method Editor
196495	QQQ Fault is not cleared when ion source is changed.
197688	Toggling triggering on/off shows misleading errors in display
198330	Acquisition Time Stamps not always recorded at start of data acquisition

2.3 Optimizer

Team Track #	Title

179062	Optimizer fails to run optimization when acquisition engines weren't running
180150	Importing from Excel spreadsheet in Optimizer got into strange state
180731	If Fragmentor coarse range is set from (0) to (any number), proper scan segments are not created.
181082	Optimizer for Peptides might not see custom modifications if the user has multiple versions of Qual
184077	Results are empty, could not obtain optimized ions for multi-compound run error when any compound RT is outside run-time of method
184209	Cannot delete method from compound setup
184570	Optimization study failed, 'input string was not in correct format'
185003	Optimizer does not run because max concurrent MRMs >200
191926	Source and iFunnel Optimizer does not support compliance
192242	Import of compounds from Acquisition method into Optimizer forces pos/neg compounds to single polarity

2.5 Study Manager

Team Track #	
162619	Multiple charge states not handled correctly via Study Manager
186264	Study manager optimizer Optimizing charge states +1, 2 and 3 when only +2 and +3 selected!
191515	AgtVoyAcqEng crashes after entering a data file path that results in a full data path longer than 256 characters

2.6 Reports

Team Track #	Title
184994	"Quant analysis script for single sample not installed..." error

3. Known Problems Detailed Description

The following is the detailed descriptions of the known problems in the QQQ software. This section includes more extensive information from our defect tracking database. This section also includes any known workarounds or recovery paths.

3.1 Tuning

Team Track # 180007	
Title	Clicking on the Tune file Browse button, brings up worklist select instead
Description	In Acquisition, QQQ tab, on the left panel, in the Tune files section, clicking on the "Browse" button brings up a file select box for worklists instead.
Workaround	Browser to <Customer Home>\Tune\QQQ\<Model #>

Team Track # 183592	
Title	Method pane type mismatch exception after switching back from Tune context and trying to load a method
Description	When I came to the system the Acquisition software was in Tune context and was locked (I could not switch back to the Acquisition context). It was locked by Study Manager which had run some worklist only studies last night. I stopped the Study

	Manager queue to unlock the Acq UI and switched back to Acquisition context. I submitted an optimization only study and noticed the source parameters did not look like they were adjusting (ex. sheath gas was set to 250 in the method, but was holding around 375), so I stopped the study. I manually loaded the method I was going to optimize with so the source temps would adjust and saw a "type mismatch" exception in the Method Pane.
Workaround	The workaround is to click on OK and you can continue

Team Track # 195805	
Title	Diverter valve error at end of autotune.
Description	The following message was displayed at the end of unit autotune: Error message "Diverter Valve set to MS during tune. Process will abort." The tune finished and reports were generated.
Workaround	Can be safely ignore

3.2 Acquisition

Team Track # 178134	
Title	Time segments not updating on DMRM run with Waste time segments
Description	When running a DMRM run (on a simulator or real instrument), the 1st time segment is always displayed in teal. Any additional time segments are not highlighted as they are run. This is only a display problem.
Workaround	Can be safely ignored

Team Track # 185743	
Title	"Script Help" tab in scripts don't have required information.
Description	Steps: 1.Open scripts dialog and select a. "ClearTrace" Observation: In script help, only "clear trace" is mentioned. Resolution: "Location" or "Trace file name" needs to be mentioned in the parameter text box. b. "LCCondition" Observation: In script help; only "Load a method is mentioned”. It does not give error if method is not mentioned in parameter. Resolution: Need to show that "Method name" or "location" needs to be mentioned in parameter
Workaround	

Team Track # 191617	
Title	6490 tune file loaded on 6460 instrument will not allow parameters to be downloaded to instrument
Description	User put a 6490 tune file on a 6460 and tries to download the method to the instrument; the device driver goes into 'downloading set points to the instrument' state.
Workaround	Do not share tune files between different models

Team Track # 193725	
Title	Run parameter error fault in MS.

Description	Got an MS fault - Run parameter error. The logbook says that the fault was cleared, but the MS stayed offline. Had to recycle power on the MS to get it back online.
Workaround	Clear fault in Tune. If fails then power cycle the MS

Team Track # 194801	
Title	Run acquisition with wrong ion source in method got software into hung state
Description	I was running on a simulator as a 6490 with AJS. I clicked New Method and Run (right together) and then realized I hadn't changed the ion source in the method to match the instrument. I clicked Stop to fix the source mismatch, but then the UI got into a hung state where the run buttons were all disabled. I had to kill all processes to restart.
Workaround	Run Remove MassHunter Process. Check the Method before running.

Team Track # 196037	
Title	Slightly different peptides with same transitions and different RTs lead to only first peptide being collected
Description	We have a few peptides that have the SAME Q1/Q3 values for several transitions and the peptides elute closely chromatographically. We're using dMRM with 3 minute windows. What should happen when we have two identical Q1/Q3 transitions with different retention times? I've seen data where it starts with the earlier eluting instance, collects for 3 minutes, and then drops it. In our case, our identical transitions with different RTs elute so closely that they overlap for a RT range (~1min?).
Workaround	To get around it, we've been calculating the average RT between the two peptides and putting in an extra wide RT window to cover both.

Team Track # 196471	
Title	CE defined in Acq Method is not acquired when you look at data file
Description	Acquired data shows one CE collected properly, but the other is at 0V. For quick reference, the transition of question in this data file is 356 -> 185, and should have both a 12V and 16V CE. Only 12V is present in the data, but data acquisition method appears correct.
Workaround	

Team Track # 196476	
Title	iFunnel parameters will not be set from tune file values in Offline Method Editor
Description	In the online UI, the iFunnel parameters are read from the tune file when creating a new method or loading an old method in which the iFunnel values were not previously set. The values are retrieved from the tune file. However, in the Offline Method Editor we are not able to get the Tune file values. When doing a new Method in offline mode, the iFunnel parameters will be set as 150/60 for both positive and negative.
Workaround	Load method online and then adjust IFunnel parameters if necessary. Right click/Default will select tune values.

Team Track # 196495	
Title	QQQ Fault is not cleared when ion source is changed.
Description	1) Had an MMI source installed. Put the MS in standby mode, then switched to AJS _ESI source. QQQ faults were generated but got cleared and were able to turn on the MS. 2) Again put MS in Standby and switched back to MMI source. Again faults were

	generated and were able to turn on MS. 3) With MS in Standby, installed the AJSESI source. This time, fault did not get cleared and the MS was offline.
Workaround	Go into Tune and click clear fault. If that doesn't work then power cycle the MS.

Team Track # 197688	
Title	Toggling triggering on/off shows misleading errors in display
Description	Starting with a triggering method, I toggled the triggering off to run with only the primaries. This produced a display indicating there were errors in the method that need to be corrected. However, the method can be saved, and the error indicators are cleared. The saved method runs fine. Turns out, clicking <apply> after turning off the triggering also clears the errors. It appears that the indication of errors is benign but misleading, and some users may start editing their method when in fact there is nothing wrong with it. Not sure if this is specific to this pos/neg method
Workaround	Click <Apply> when switching between DMRM and TMRM

Team Track # 198330	
Title	Acquisition Time Stamps not always recorded at start of data acquisition
Description	A worklist was acquired with overlapped injection. Run time was set for 12 min. Acquisition time stamp differences between consecutive samples should be around 12 min. It was found to be around 12min 30 seconds for some samples, but some only was 30 seconds and others 24min 30 seconds. This seems to indicate that the recording time is not always at the start of the data acquisition.
Workaround	

3.3 Optimizer

Team Track # 179062	
Title	Optimizer fails to run optimization when acquisition engines weren't running
Description	I ran Optimizer (which starts the engines), created a project, and tried to Optimize a mass. As soon as the optimization run started I got an error saying "Error occurred during optimization. Device: MSQQQ_1 for operation: PrepareRun failed Phase 2: Optimization failed". I had not run the Acq UI, so I suspect Optimizer starting engines and running without the Acq UI led to something not getting initialized properly in the QQQ.
Workaround	Run Acq UI first before starting Optimizer

Team Track # 180150	
Title	Importing from Excel spreadsheet in Optimizer got into strange state
Description	In process to set up a project from one of the Excel spreadsheets, after the spreadsheet has been imported, the Compound Setup tab got into a very strange state. The header names were all the internal names, internal IDs were seen, and the checkbox column was not working.
Workaround	Restart the Optimizer software and start with clean project

Team Track # 180731	
Title	If Fragmentor coarse range is set from (0) to (any number), proper scan segments are

	not created.
Description	Steps: 1. Launch Optimizer and create a new project. 2. Set Fragmentor coarse range from (0) to (20) 3. Fill other required parameters and start optimization Observation: Only 2 Scan Segments are created one with fragmentor value as (0) and other with fragmentor value as (1). Ideally six scan segments should have got created Note: Observed only when Start of range is Zero.
Workaround	Avoid starting Fragmentor range with zero.

Team Track # 181082	
Title	Optimizer for Peptides might not see custom modifications if the user has multiple versions of Qual installed.
Description	If the customers have multiple version of Qual installed, Optimizer will not know which Qual directory to look for customer modifications.
Workaround	Need to transfer all custom modifications to latest Qual.

Team Track # 184077	
Title	Results are empty, could not obtain optimized ions for multi-compound run error when any compound RT is outside run-time of method
Description	A method was created with one-minute run time. In Optimizer, 321 and 621 masses were added. Then, RT/RT window values of 3/0.2 for 321 and 0.5/0.2 for 621 are added and a multi-compound DMRM optimization was run. When optimization finished the error message was displayed: "Error occurred during optimization. Results are empty, could not obtain optimized ions for multi-compound run."
Workaround	Make sure RT is set correctly

Team Track # 184209	
Title	Cannot delete method from compound setup
Description	In compound setup, select perform multi-compound run, add a compound, add a method and before you enter precursor/product ion info add a method again. However, when you try to delete the second method, you get the following error: "All selected rows cannot be deleted. For multi compound run, each selected compound should have at least one product ion”
Workaround	Enter precursor/product ion information for the first method before deleting the second method

Team Track # 184570	
Title	Optimization study failed, 'input string was not in correct format'
Description	Optimization only study failed. The error message was "Optimization error. Input string was not in a correct format. Couldn't store <1.019147E+07> in Abundance Column. Expected type is Decimal." This message came at the end of optimization. However, the logbook also showed that all four compounds were optimized 100%. Qual data showed peaks in the P2 phase were all 10 times more abundant than the P3 and P4 peaks.
Workaround	Reduce injection volume

Team Track # 185003	
Title	Optimizer does not run because max concurrent MRMs >200
Description	If the CE values are deleted and then multi-compound/DMRM optimization is started then optimizer will not run and the message "Optimization stopped" popped up.
Workaround	None

Team Track # 191926	
Title	Source and iFunnel Optimizer does not support compliance
Description	Source and iFunnel Optimizer does not support compliance. Currently, Source and iFunnel Optimizer will create Quant batch, Quant method, and an Excel Quant report without using user login information. If Quant compliance was supported, the Quant compliance user login information (user ID and password) have to be used in Source and iFunnel Optimizer.
Workaround	

Team Track # 192242	
Title	Import of compounds from Acquisition method into Optimizer forces pos/neg compounds to single polarity
Description	I took a functioning pos/neg Acquisition method and imported it into Optimizer. It appears that upon import, all ion polarities are forced to a single polarity, I'm guessing corresponding to the polarity of the first compound (in this case, negative). This has the consequence that all the positive mode compounds in my method are converted to negative mode compounds...not what I wanted. The only way I can figure to work around this problem is to segregate my pos/neg method first into pos-only and a neg-only methods, and then import--actually didn't take very long because one can sort by polarity in the Acq method.
Workaround	Before importing to Optimizer, create two versions of the method, one for each polarity. Sort the compounds by polarity and delete the positive or negative transitions before saving each method.

3.4 Study Manager

Team Track # 162619	
Title	Multiple charge states not handled correctly via Study Manager
Description	Optimizer from Study Manager does not behave correctly when +1 and +2 charge states were selected in the Project. Check box for most abundant is selected but the product ion scan step is always done based on the charge state on the top of the list. Optimizer behaves correctly when standalone was run.
Workaround	Recommend to use peptide optimizer or Skyline.

Team Track # 186264	
Title	Study manager optimizer Optimizing charge states +1, 2 and 3 when only +2 and +3 selected!
Description	Set up a BSA method on a C8 column for optimizer. Charge states +2 and +3 were selected for the parent ion 1443.61. Optimizer was run and 722.816 and 482.21 were determined to be the +2 and +3 states, eventually 482.21 was determined to be most abundant, etc. In same optimization called from Study Manager adds 1443.61, 722.816 and 482.21 to the first table of MS2SIM ions to optimize. Charge state 1 is not selected

	but was included.
Workaround	Recommend to use peptide optimizer or Skyline.

Team Track # 191515	
Title	AgtVoyAcqEng crashes after entering a data file path that results in a full data path longer than 256 characters
Description	Created a path that was 235 characters long: C:\MassHunter\Studies\longpathtest\longpathtest1\longpathtest2\longpathtest3\longpathtest4\longpathtest5\longpathtest6\longpathtest7\longpathtest8\longpathtest9\longpathtest10\longpathtest11\longpathtest12\longpathtest13\longpathtest14. When I submitted a data file name of 'Sample0007.d' and a method name of MM6460ESINeg.M, acquisition crashed.
Workaround	Avoid long study, project, and method names.

3.5 Reports

Team Track # 184994	
Title	"Quant analysis script for single sample not installed..." error
Description	I changed the <Customerhome> folder from D:\MassHunter to D:\QQQ. I copied methods and worklist from D:\MassHunter to corresponding folders on D:\QQQ and changed method and data path in the worklist. I also changed the Quant DA method path in the method editor to reflect D:\QQQ\methods...I started the worklist. It stopped after the first sample with the message "Quant analysis script for single sample not installed" I also tried to change the method and data path in worklist parameters to D:\QQQ but I was unable to save the method, the error message was "there is an error in the worklist" and there was no more information.
Workaround	

Appendix A. Glossary

Term / Acronym	Definition
QQQ	Triple Quadrupole instrument.
UI	User Interface. The visual representation of the software with which a user interacts.
MRM	Multiple Reaction Monitoring
DMRM	Dynamic MRM
TMRM	Triggered MRM
VWD	Variable Wavelength Detector
CE	Collision Energy
MS	Mass Spectrometer
RT	Retention Time
MMI	Multimode Interface