
Software Release Bulletin

MassHunter Qual MassHunter Qual B.06.00 SP1

Apr 10 2013 9:56AM

Preface

This Software Release Bulletin documents all fixes and enhancements that are incorporated the new release.

Keyword Glossary

Keyword Index

KPR#: 14416 Product: MassHunter Qual MassHunter Qual B.06.00

Keyword:

One-line Description:

Translated LC/MS ChemStation files cause exception and do not load

Problem:

- 1) Open any LC/MS SQ file, such as "mssulfas.d"
- 2) Newly translated ChemStation LC/MS files causes the exception:
 "Opening datafile failed with error - Unsupported element type in schema file."

Occurs with the current release of LC/SQ Translator B.04.00 (B481.9)

Note: all sample files open without error in B.05.00 SP1 (519.13)
Translated GC-MS files also have no problem.

Temporary Solution:

n/a

Fix Information:

n/a

KPR#: 14417 Product: MassHunter Qual MassHunter Qual B.06.00

Keyword:

One-line Description:

For Find by All Ions MSMS the Confirm with "average fragment spectrum" will not work unless a suitable PCD.CDB or PCDL.CDB is specified in Formula Source

Problem:

Neither manual entry of formulas in the FbyF UI nor a CSV database can be successfully used as a formula source for All Ions MSMS where fragment confirmation is set to "average fragment spectrum". This results in "No compounds found". The source must be a CDB file.

Temporary Solution:

n/a

Fix Information:

n/a

KPR#: 14418 Product: MassHunter Qual MassHunter Qual B.05.00 SP1

Keyword:

One-line Description:

A cef file loaded into Qual without Bioconfirm will not display the "Sequence Name," "Sequence", and "Type."

Problem:

- Load a cef file with sequence information into Qual without Bioconfirm.
- The columns for "Sequence Name," "Sequence" and "Type" will be blank.

Temporary Solution:

n/a

Fix Information:

n/a

KPR#: 14419 Product: MassHunter Qual MassHunter Qual B.05.00 SP1

Keyword:

One-line Description:

Swiss-prot ID is not being read from a .cef file into Qual

Problem:

- Swiss-prot ID's are currently not being read into Qual from a .cef file.
- The columns in Qual are blank.

Temporary Solution:

n/a

Fix Information:

n/a

KPR#: 14420 Product: MassHunter Qual MassHunter Qual B.05.00 SP1

Keyword:

One-line Description:

Increase RT tolerance in DBSearch & FbF

Problem:

Retention time tolerance limits need to be set from 0 - 1000.

Temporary Solution:

n/a

Fix Information:

n/a

KPR#: 14422 Product: MassHunter Qual MassHunter Qual B.06.00

Keyword:

One-line Description:

BioConfirm OligoNucleotide report template throws RPC exception with Excel 2013 and add-in.

Problem:

BioConfirm OligoNucleotide report template throws RPC exception with Excel 2013 and add-in.

Temporary Solution:

n/a

Fix Information:

n/a

KPR#: 14423 Product: MassHunter Qual MassHunter Qual B.06.00

Keyword:

One-line Description:

Attempting to generate Qual B.06 reports to PDF results in an exception with Excel2013 and an add-in

Problem:

Attempting to generate Qual B.06 reports to PDF results in an exception with Excel2013 and an add-in.

Temporary Solution:

n/a

Fix Information:

n/a

KPR#: 14424 Product: MassHunter Qual MassHunter Qual B.06.00

Keyword:

One-line Description:

Allions -- A qualified fragment ion without coelution score

Problem:

Steps to reproduce:

Datafile: Cal_09-r002.d

DataSource: Pesticides_AM_PCDL.cdb

Method: default.m and override the datasource.

Run FbF with FragmentConfirmation checked.

Cpd9:Hymecromome(RT=7.225) has one qualified frag ion mz=121.06.

Its coelution score is empty in the fragment ion table.

Temporary Solution:

n/a

Fix Information:

n/a

KPR#: 14425 Product: MassHunter Qual MassHunter Qual B.06.00

Keyword:

One-line Description:

CF = 0, DF = 0 are visible in both chromatogram and spectra results panes

Problem:

-Chromatogram and Spectra Results panes will display: CF = 0.000 and DF = 0.000 at the top.

-This is a FAIMS feature that has not been implemented yet.

Temporary Solution:

n/a

Fix Information:

n/a

KPR#: 14426 Product: MassHunter Qual MassHunter Qual B.06.00

Keyword:

One-line Description:

DB Search is not correctly updating the combined result and the best result when preceded by other operations.

Problem:

-FbF + MFG + DB Search(Library search) will change the "best" results of a compound.

Temporary Solution:

n/a

Fix Information:

n/a

KPR#: 14427 Product: MassHunter Qual MassHunter Qual B.06.00

Keyword:

One-line Description:

If Windows was installed with a language setting that is NOT US English, Simplified Chinese, or Japanese, a Qual B.06 installation will fail

Problem:

If Windows was installed with a language setting that is NOT US English, Simplified Chinese, or Japanese, a Qual B.06 installation will fail and generate a "Installation has ended prematurely" error.

Temporary Solution:

n/a

Fix Information:

n/a

KPR#: 14428 Product: MassHunter Qual MassHunter Qual B.06.00

Keyword:

One-line Description:

Exception thrown when printing FbF compound reports with library spectrum or difference plot checked

Problem:

Launch Qual B.06.00
Run Find Compounds by Formula;
Run Identify Compounds -> Search Database;

and Identify Compounds -> Search Accurate Mass Library
Print compound report

The following exception is thrown:

Date and Time: 3/27/2013 4:28 PM

Program: Agilent MassHunter Workstation Software Qualitative Analysis B.06.00

Build Configuration: Release

Message: Value cannot be null.

Parameter name: targetSpec or resultSpec cannot be null

Stack Trace:

Server stack trace:

```
    at
Agilent.MassSpectrometry.DataAnalysis.Qualitative.QualPlotControl.Agilent.MassSpectrometry.DataAnalysis.C
targetSpec, ISpectrum resultSpec, ISpectrum targetMSMSSpec)
    at
Agilent.MassSpectrometry.DataAnalysis.Qualitative.BaseReportGenerator.CreateLibrarySpectrumPerHit(IData
dataltem, ExportedImageType imageType, ISpectralLibrarySearchHit hitObject, Boolean
showLibrarySpectrum, Boolean showDifferenceSpectrum, String& libSpecFilePath, String& specDiffFilePath)
    at
Agilent.MassSpectrometry.DataAnalysis.Qualitative.BaseReportGenerator.WriteLibrarySearchResults(IDatalte
dataltem, Boolean showLibrarySpectrum, Boolean showDifferenceSpectrum)
    at
Agilent.MassSpectrometry.DataAnalysis.Qualitative.CompoundReportGenerator.WriteCompounds(IDataltem[]
compounds)
    at
Agilent.MassSpectrometry.DataAnalysis.Qualitative.CompoundReportGenerator.GenerateReportSpecialized(II
selectedAnalysis)
    at
Agilent.MassSpectrometry.DataAnalysis.Qualitative.BaseReportGenerator.GenerateReportAndMapExceptions
analyses)
    at Agilent.MassSpectrometry.DataAnalysis.Qualitative.BaseReportGenerator.GenerateReport(IDataltem[]
selectedAnalysis)
    at Agilent.MassSpectrometry.DataAnalysis.Qualitative.CmdGenerateReport.DoSpecialized()
    at Agilent.MassSpectrometry.DataAnalysis.Qualitative.QualCommandBase.Do()
    at Agilent.MassSpectrometry.CommandModel.CommandHistory.Invoke(ICommand cmd)
    at System.Runtime.Remoting.Messaging.StackBuilderSink._PrivateProcessMessage(IntPtr md, Object[]
args, Object server, Int32 methodPtr, Boolean fExecuteInContext, Object[]& outArgs)
    at
System.Runtime.Remoting.Messaging.StackBuilderSink.PrivateProcessMessage(RuntimeMethodHandle
md, Object[] args, Object server, Int32 methodPtr, Boolean fExecuteInContext, Object[]& outArgs)
    at System.Runtime.Remoting.Messaging.StackBuilderSink.AsyncProcessMessage(IMessage msg,
IMessageSink replySink)
```

Exception rethrown at [0]:

```
    at System.Runtime.Remoting.Proxies.RealProxy.EndInvokeHelper(Message reqMsg, Boolean
bProxyCase)
    at System.Runtime.Remoting.Proxies.RemotingProxy.Invoke(Object NotUsed, MessageData& msgData)
    at Agilent.MassSpectrometry.CommandModel.CommandHistory.InvokeCommand.EndInvoke(IAsyncResult
result)
    at Agilent.MassSpectrometry.DataAnalysis.Qualitative.AppManager.EndInvoke(IAsyncResult result)
```

at Agilent.MassSpectrometry.DataAnalysis.Qualitative.QualForm.OnAsyncCallBack(IAAsyncResult
asyncResult)

Temporary Solution:

n/a

Fix Information:

n/a

KPR#: 14429 Product: MassHunter Qual MassHunter Qual B.06.00

Keyword:

One-line Description:

Reporting fails when processing worklist

Problem:

When processing worklist of 25 entries (via Worklist Automation), reporting failures occur and reports are intermittently lost.

Temporary Solution:

n/a

Fix Information:

n/a

KPR#: 14430 Product: MassHunter Qual MassHunter Qual B.06.00

Keyword:

One-line Description:

Structures imported from ChemSpider appear with zigzag bonds

Problem:

A .mol file for a compound from ChemSpider will show the bonds as zig-zag lines instead of straight lines in both PCDL Manager and Qual.

Temporary Solution:

n/a

Fix Information:

n/a