

Version

C

LEOSON BV

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QuantBrowser startershandbook

LEOSON BV

Product manual

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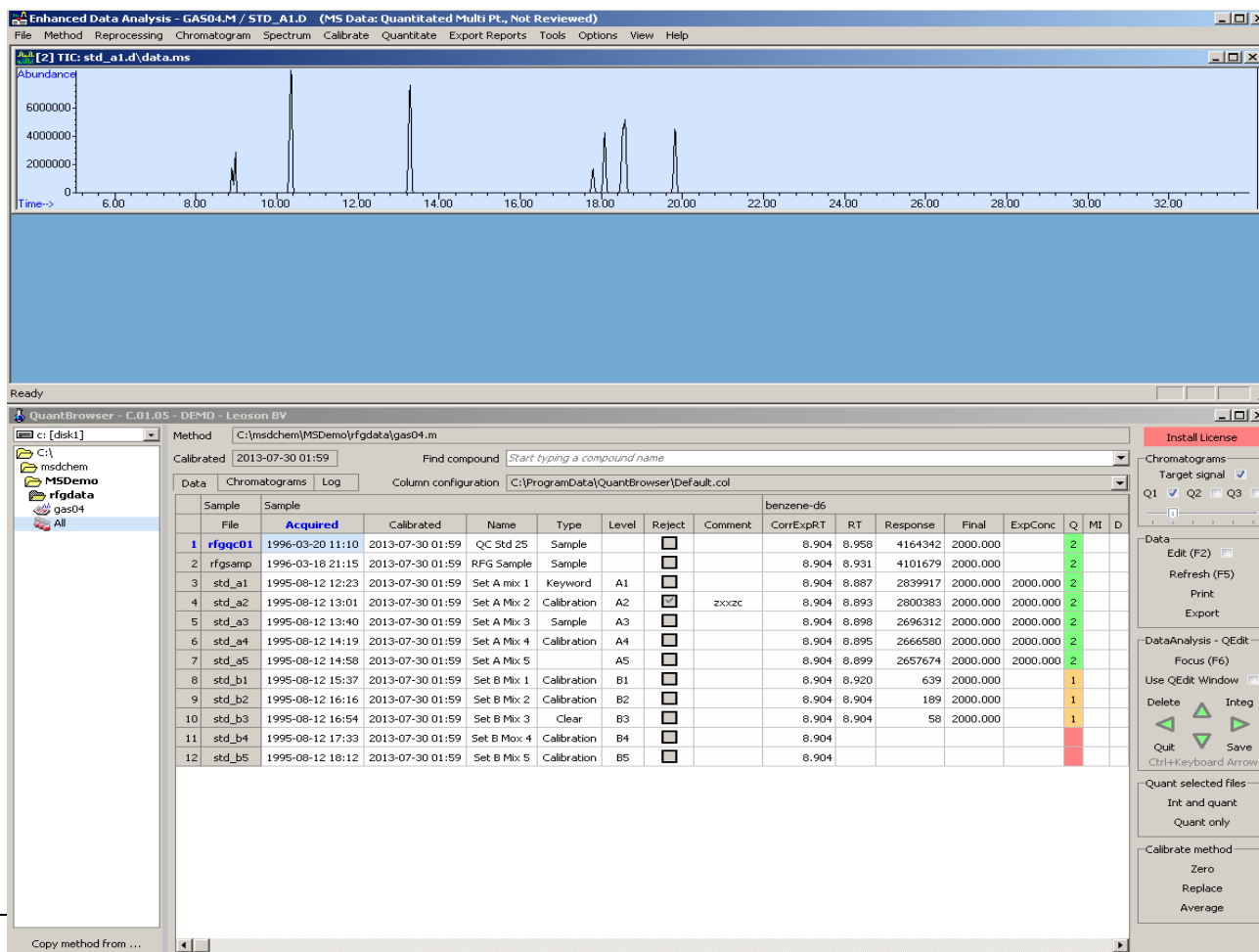
Introduction

Concept

QuantBrowser is an integrated add-on to Agilent DataAnalysis.

DataAnalysis operates on single samples with functions like Quantitation, Calibration, Reporting and QEdit.

QuantBrowser operates on a complete sequence. The results are displayed in a excel-like sheet, as shown in an example below.







Supported platform

The platforms that support QuantBrowser are Agilent GCMS ChemStation C.00-E.02

Installation

To install QuantBrowser, execute the QuantBrowserSetup.exe. Additional files that are stored in the same folder are automatically installed by the setup program. The additional files are Column configuration files (.col) and a license file (.lic).

 Concentration.col	8/28/2013 5:46 PM	COL File
 Default.col	8/28/2013 5:25 PM	COL File
 QuantBrowserSetup.exe	8/28/2013 6:03 PM	Application
 RetentionTime.col	8/28/2013 5:45 PM	COL File



Launch

To launch QuantBrowser, double-click the desktop shortcut or click the integrated toolbutton (#1) in Agilent DataAnalysis.



License

Install the license file to unlock demo mode. A license file can be obtained through www.walson.eu.

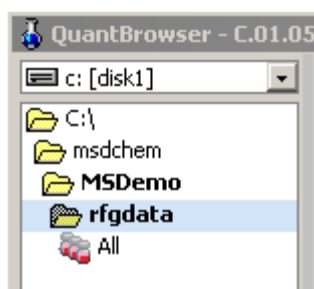


Chapter
2

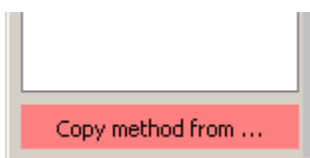
Quick Start

Prepare a dataset

1. Navigate to the data folder



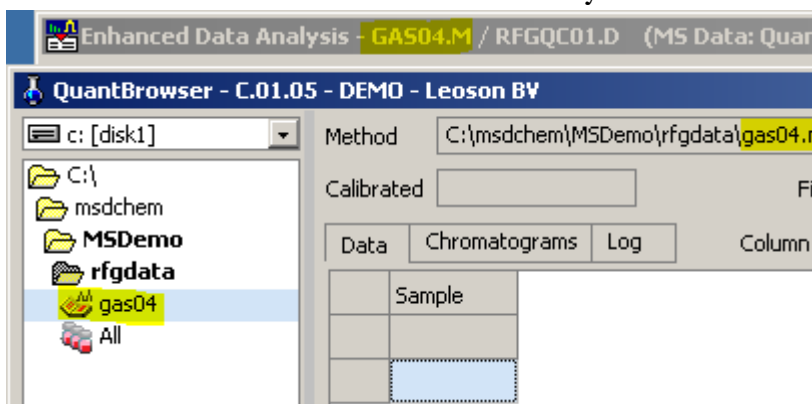
2. Copy a method to the data folder



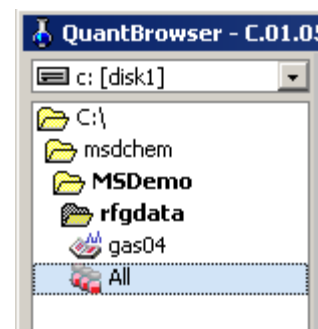
3. Load the method in DataAnalysis, double-click on the method



4. Find the loaded method name in DataAnalysis title



5. List the samples and results, double click on All



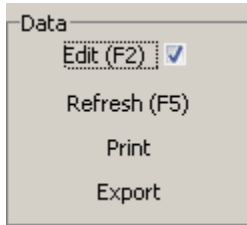
QUANTBROWSER FOR AGILENT GCMS CHEMSTATION

6. Find the samples and results in the table

	Sample	Sample							benzene-d6						
	File	Acquired	Calibrated	Name	Type	Level	Reject	Comment	Response	Final	ExpConc	Accuracy	Q	MI	D
1	rfgqc01	1996-03-20 11:10	2013-07-30 01:59	QC Std 25			<input type="checkbox"/>		4164342	2000.000			2		
2	rfgsamp	1996-03-18 21:15	2013-07-30 01:59	RFG Sample			<input type="checkbox"/>		4101679	2000.000			2		
3	std_a1	1995-08-12 12:23	2013-07-30 01:59	Set A mix 1			<input type="checkbox"/>		2839917	2000.000			2		
4	std_a2	1995-08-12 13:01	2013-07-30 01:59	Set A Mix 2			<input type="checkbox"/>		2800383	2000.000			2		
5	std_a3	1995-08-12 13:40	2013-07-30 01:59	Set A Mix 3			<input type="checkbox"/>		2696312	2000.000			2		
6	std_a4	1995-08-12 14:19	2013-07-30 01:59	Set A Mix 4			<input type="checkbox"/>		2666580	2000.000			2		
7	std_a5	1995-08-12 14:58	2013-07-30 01:59	Set A Mix 5			<input type="checkbox"/>		2657674	2000.000			2		
8	std_b1	1995-08-12 15:37	2013-07-30 01:59	Set B Mix 1			<input type="checkbox"/>		639	2000.000			1		
9	std_b2	1995-08-12 16:16	2013-07-30 01:59	Set B Mix 2			<input type="checkbox"/>		189	2000.000			1		
10	std_b3	1995-08-12 16:54	2013-07-30 01:59	Set B Mix 3			<input type="checkbox"/>		58	2000.000			1		
11	std_b4	1995-08-12 17:33	2013-07-30 01:59	Set B Mox 4			<input type="checkbox"/>								
12	std_b5	1995-08-12 18:12	2013-07-30 01:59	Set B Mix 5			<input type="checkbox"/>								

Calibrate

1. Edit sample type and level



2. Set calibration levels, right click in level column

Type	Level
Control	
Sample	
Calibration	A1
Calibration	A2
Calibration	A3
Calibration	A4
Calibration	A5
Calibration	B1
Calibration	B2
Calibration	B3
Calibration	B4
Calibration	B5

Load data file	
Copy	Ctrl+C
Windows explorer	Ctrl+E
Integrate and quantitate selected datafiles	
Quantitate selected datafiles	
Batch editor ...	
Add to batch ...	
Remove from batch	
Delete batch ...	
Clear	
A1	
A2	
A3	
A4	
A5	
B1	
B2	
B3	
B4	
B5	

The image shows a table with two columns: "Type" and "Level". The "Level" column contains calibration levels A1 through B5. A red arrow points to the "B4" level in the "Level" column. To the right of the table is a context menu titled "Load data file" with various options including "Copy", "Windows explorer", "Integrate and quantitate selected datafiles", "Quantitate selected datafiles", "Batch editor ...", "Add to batch ...", "Remove from batch", "Delete batch ...", "Clear", and a list of calibration levels (A1 through B5). The "B5" option in the list is highlighted in blue.

3. Set sample type, right click in type column

Type	Level	Reject	Comment
Control		<input type="checkbox"/>	
Sample		<input type="checkbox"/>	
Calibrat			

Load data file	
Copy	Ctrl+C
Windows explorer	Ctrl+E
Integrate and quantitate selected datafiles	
Quantitate selected datafiles	
Batch editor ...	
Add to batch ...	
Remove from batch	
Delete batch ...	
Clear	
Sample	
Blank	
Calibration	
Negative	
Control	
Keyword	
BFB	
DFTPP	

4. Select all samples, click in upper left corner

Data		Chromatograms	Log
+	Sample	Sample	
	File	Acquired	
1	rfgqc01	1996-03-20 11:10	20
2	rfgsamp	1996-03-18 21:15	20

5. Integrate and quantitate selected samples

	Sample	Sample				
	File	Acquired	Calibrated	Name	Type	Lev
1	rfgqc01	1996-03-20 11:10	2012-07-20 01:50	GC STD 25	Control	
2	rfgsamp	1996-03-1				
3	std_a1	1995-08-1				
4	std_a2	1995-08-1				
5	std_a3	1995-08-1				
6	std_a4	1995-08-1				
7	std_a5	1995-08-1				
8	std_b1	1995-08-1				
9	std_b2	1995-08-1				

Load data file	
Copy	Ctrl+C
Windows explorer	Ctrl+E
Integrate and quantitate selected datafiles	
Quantitate selected datafiles	
Batch editor ...	
Add to batch ...	
Remove from batch	
Delete batch ...	

6. Zero all responses in the calibration table, click on Zero

Calibrate method
Zero
Replace
Average

7. Select the calibration samples

Type	Level
Control	
Sample	
Calibration	A1
Calibration	A2
Calibration	A3
Calibration	A4
Calibration	A5
Calibration	B1
Calibration	B2
Calibration	B3
Calibration	B4
Calibration	B5

8. Replace the responses in the calibration table, click on Replace

Calibrate method
Zero
Replace
Average

8. Note that samples were calculated with an older version of the calibration table

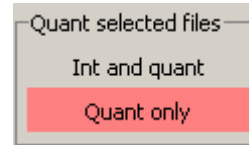
Method		C:\msdchem\MSDemo\rfgdata\gas04.m	
Calibrated		2013-08-28 20:53	Find com
Data	Chromatograms	Log	Column configu
	Sample	Sample	
	File	Acquired	Calibrated
1	rfgqc01	1996-03-20 11:10	2013-08-28 20:48
2	rfgsamp	1996-03-18 21:15	2013-08-28 20:48
3	std_a1	1995-08-12 12:23	2013-08-28 20:48
4	std_a2	1995-08-12 13:01	2013-08-28 20:48
5	std_a3	1995-08-12 13:40	2013-08-28 20:48
6	std_a4	1995-08-12 14:19	2013-08-28 20:48
7	std_a5	1995-08-12 14:58	2013-08-28 20:48
8	std_b1	1995-08-12 15:37	2013-08-28 20:48
9	std_b2	1995-08-12 16:16	2013-08-28 20:48
10	std_b3	1995-08-12 16:54	2013-08-28 20:48
11	std_b4	1995-08-12 17:33	2013-08-28 20:48
12	std_b5	1995-08-12 18:12	2013-08-28 20:48

Quantitate

1. Select all samples

Data			
Chromatograms			
Log			
+			
	Sample	Sample	
	File	Acquired	
1	rfgqc01	1996-03-20 11:10	20
2	rfgsamp	1996-03-18 21:15	20

2. Requantitate all samples, click on Quant only

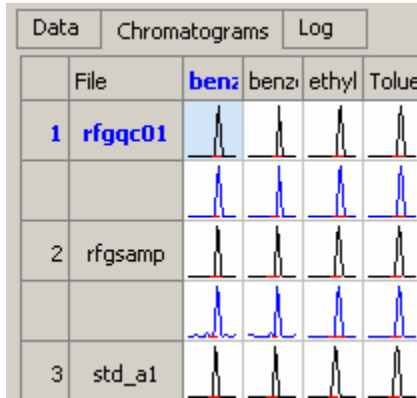


3. Note that the samples were quantitated with the current calibration table

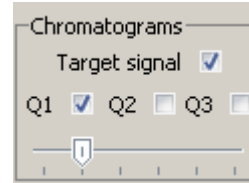
Method	C:\msdchem\MSDemo\rfgdata\gas04.m		
Calibrated	2013-08-28 20:53	Find com	
Data			
Chromatograms			
Log			
Column configu			
	Sample	Sample	
	File	Acquired	Calibrated
1	rfgqc01	1996-03-20 11:10	2013-08-28 20:53
2	rfgsamp	1996-03-18 21:15	2013-08-28 20:53

Review integration

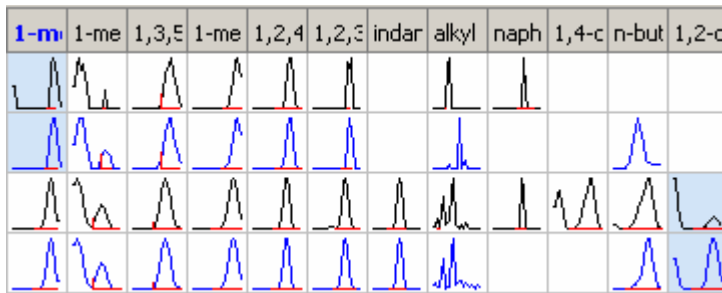
1. Review integration, click on the Chromatogram tab



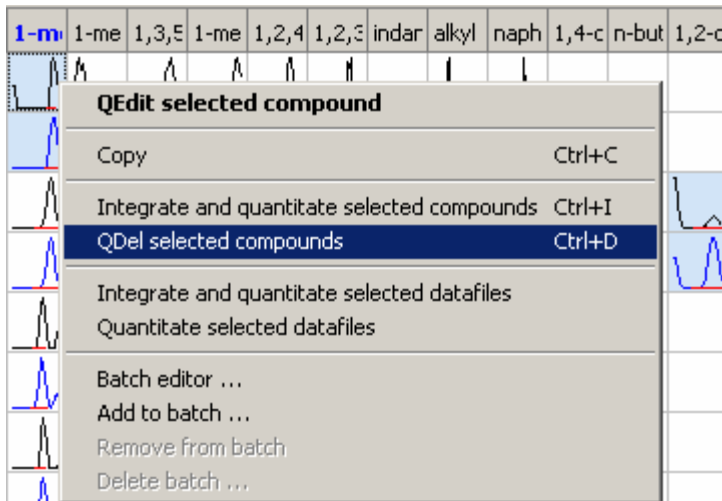
2. Select the signals and resize the plots



3. Select multiple compounds, left click while pressing the control key



4. Delete false peaks



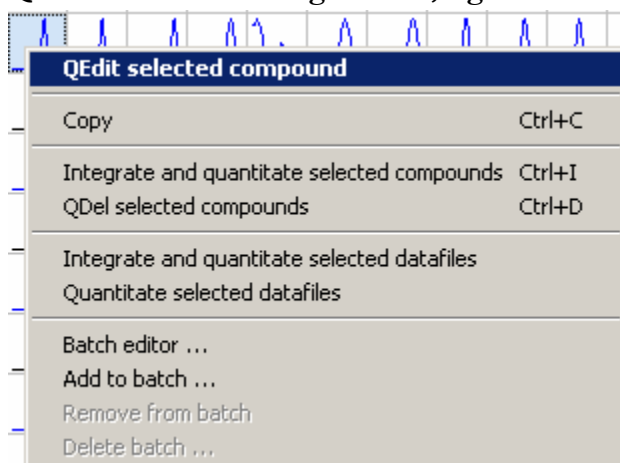
QEdit

1. Note the Response and MI value for o-xylene of std_a1

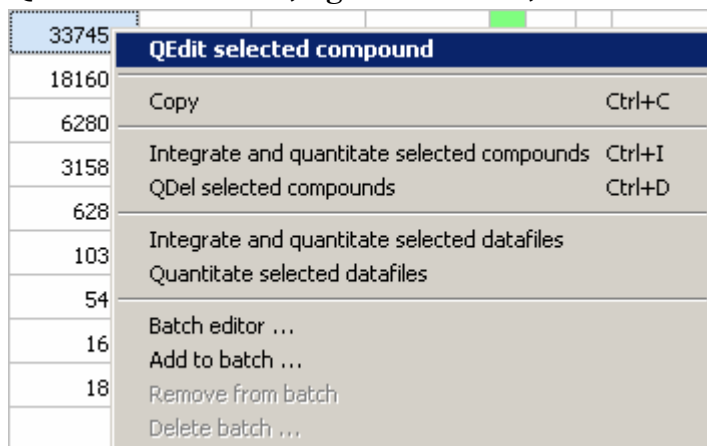
o-xylene						
Response	Final	ExpConc	Accuracy	Q	MI	D
2155357	2327.603			2		
2078636	2111.687			2		
3374554	5871.171	6000.000	97.85	2		
1816025	3218.328	3000.000	107.28	2		

2. Start QEdit

- a. QEdit from Chromatogram tab, right click menu, or double click on a plot



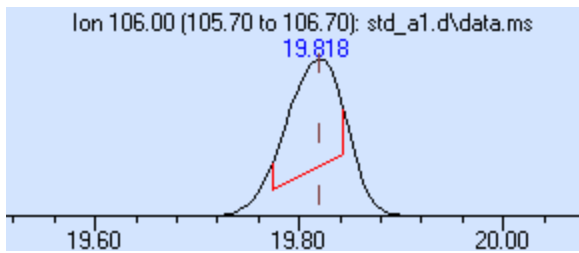
- b. QEdit from Data tab, right click menu, or double click on a compound cell



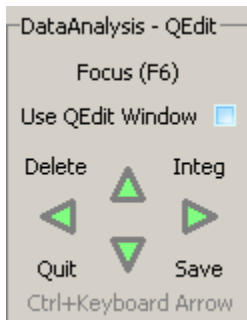
- c. QEdit with navigation arrow



3. Perform a manual integration on o-xylene of std_a1 in DataAnalysis, using the right mouse-button



4. Save QEdit in DataAnalysis, or click on navigation buttons or Save button in QuantBrowser

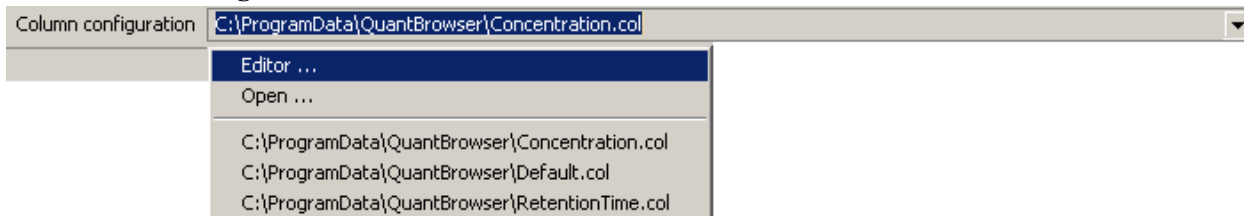


5. Note the new values for o-xylene of std_a1.

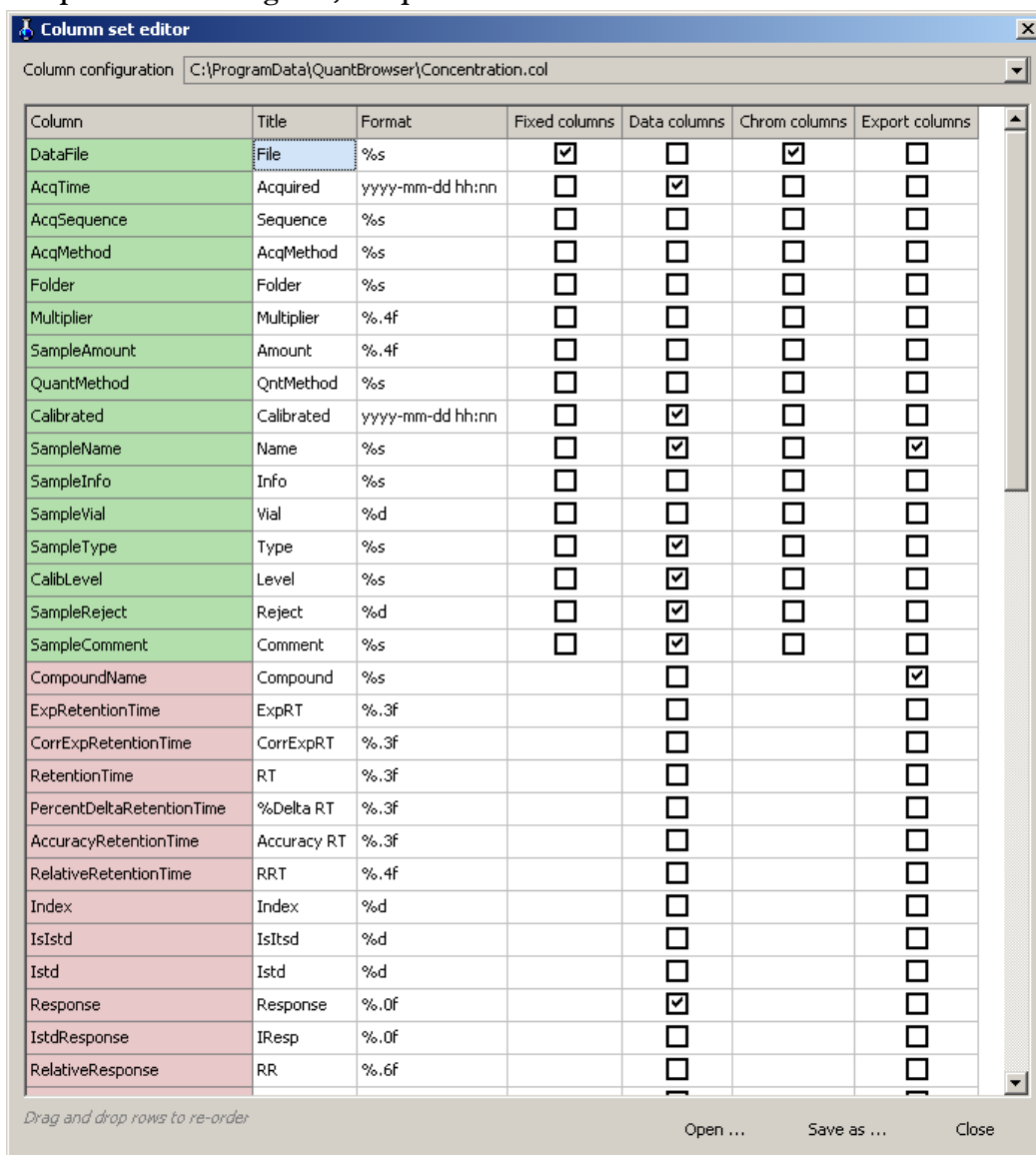
o-xylene						
Response	Final	ExpConc	Accuracy	Q	MI	D
2155357	2327.603			2		
2078636	2111.687			2		
1738070	3023.957	6000.000	50.40	1	1	
1816025	3218.328	3000.000	107.28	2		

Column configuration

1. New column configurations can be created



2. Column can be selected and re-order by drag and drop. Sample columns are green, compound columns are red.



Column information

1. Rest the mouse above a column header

		1-methylethylbenzene			
Q	MI	D	Response	Final	ExpConc
2					
2					
0	1				
8	2		5119	6.276	

Integration

0: By method

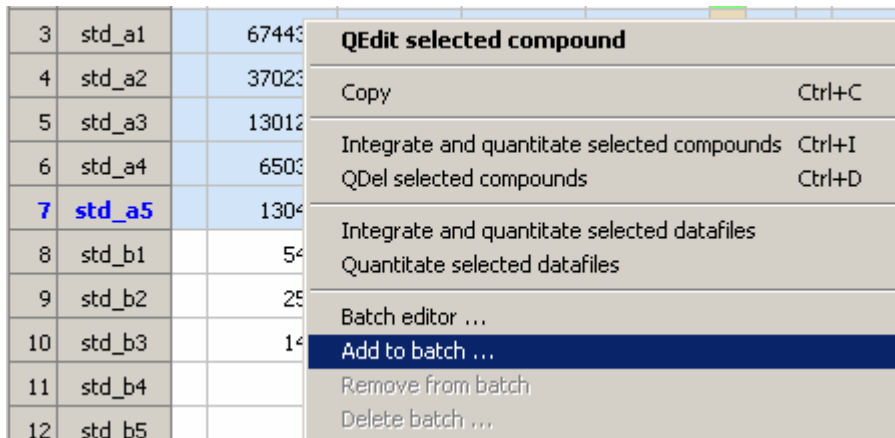
1: Manually

2: Corresponding ISTD was manual integrated

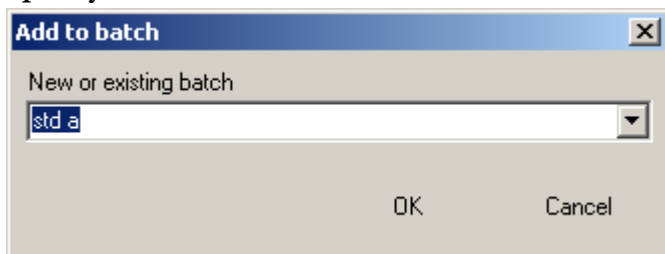
3: Both this and ISTD manual integrated

Sample batch

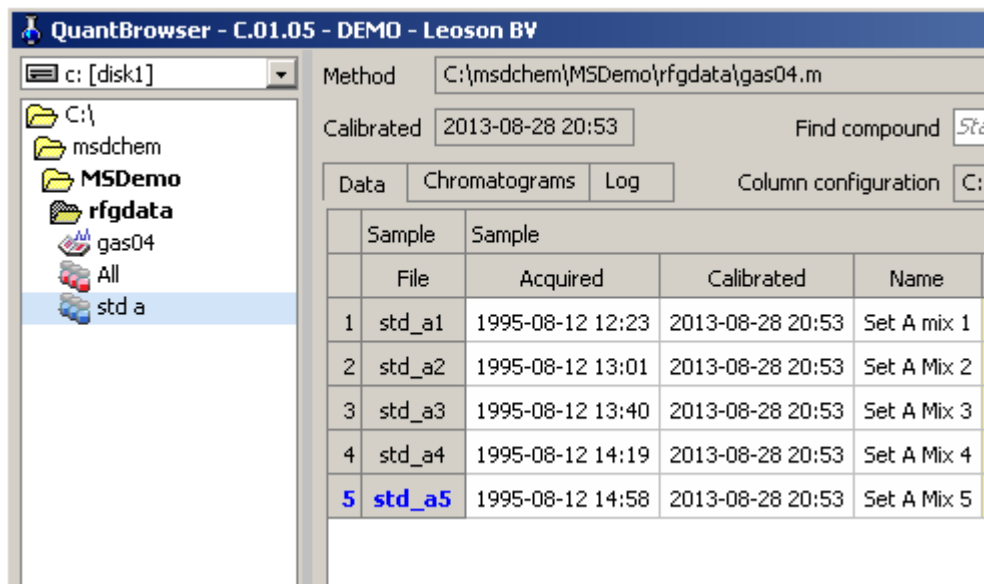
1. Select sample for the batch, right click on the samples and Add to batch



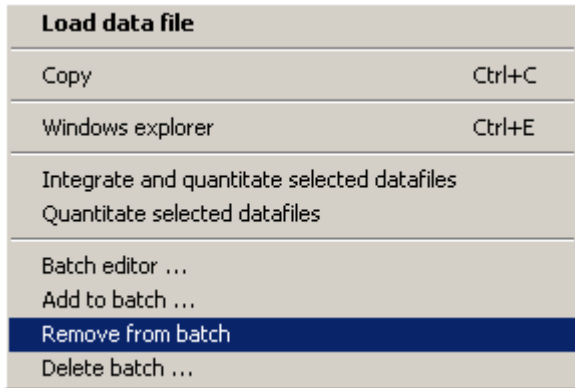
2. Specify the batch name



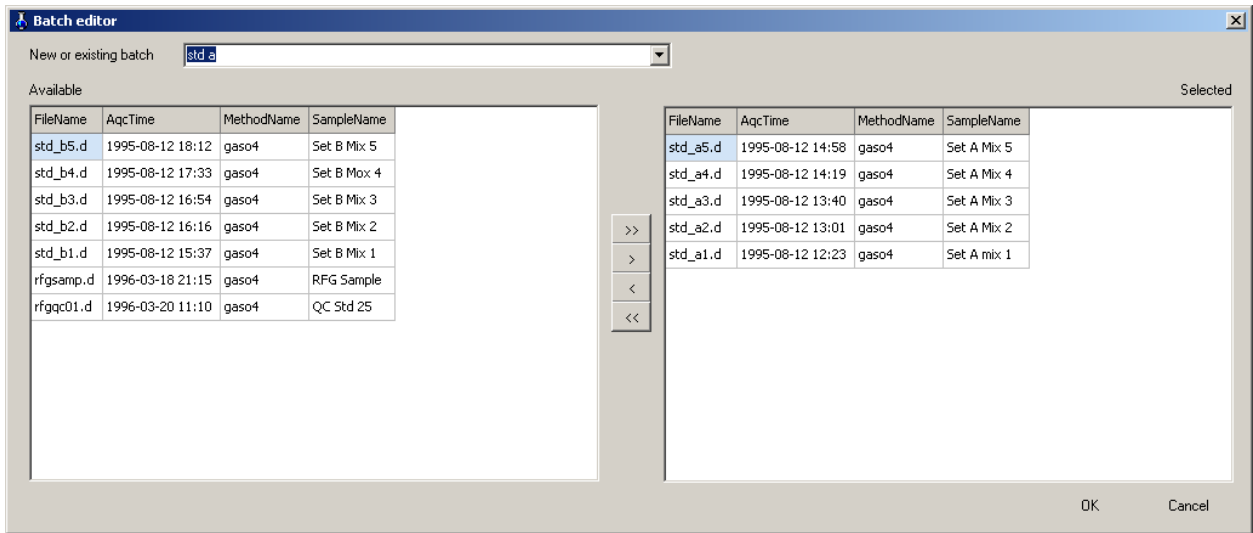
3. Find the samples in the new batch



4. Samples can be removed from the batch



5. The batch editor helps to add or remove samples, click on the column header to sort the samples

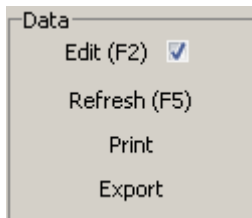


Copy to clipboard

1. Select table cells and copy to clipboard. Use the right click menu in the table.

Export data

1. Open the export dialog, click on export button



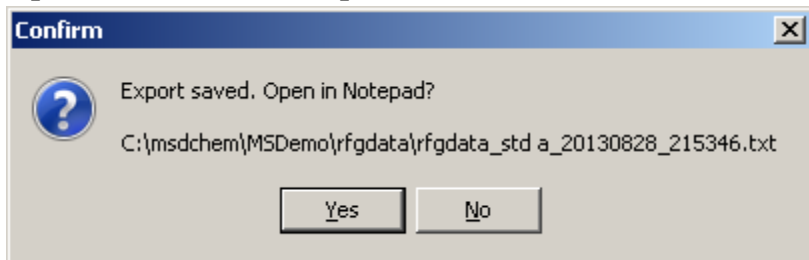
2. Specify the folder for the export file and the columns to be exported

Calibrated	Name	Type	Level	Reject	Comment	Response	Final	ExpConc
2013-08-28 20:53	Set A mix 1	Calibration	A1	<input type="checkbox"/>		2839917	2000.000	2000.000
2013-08-28 20:53	Set A Mix 2	Calibration	A2	<input type="checkbox"/>		2800282	2000.000	2000.000

A screenshot of the 'Export data' dialog box. It has the following fields and options:

- Save to:** C:\msdchem\MSDemo\rfgdata\rfgdata_std a_20130828_215346
- Save a copy to folder:** D:\LIMS GATE
- Column configuration:** C:\ProgramData\QuantBrowser\Default.col
- Export:**
 - txt
 - Exclude zero concentration
 - Exclude qualifier out of range
 - Exclude rejected samples
- Buttons:** Export, Close

3. Open the results in Notepad



4. View the results

rfgdata_std a_20130828_215346.txt - Notepad

File Edit Format View Help

Name	Compound	Final
Set A mix 1	benzene-d6	2000.000
Set A mix 1	benzene	2947.396
Set A mix 1	ethylbenzene-d10	2000.000
Set A mix 1	Toluene	13917.123
Set A mix 1	ethylbenzene	4904.068
Set A mix 1	1-methylethylbenzene	12.769
Set A mix 1	1-methyl-3-ethylbenzene	3.829
Set A Mix 2	benzene-d6	2000.000
Set A Mix 2	benzene	1527.785
Set A Mix 2	ethylbenzene-d10	2000.000
Set A Mix 2	Toluene	10753.207
Set A Mix 2	ethylbenzene	2660.650
Set A Mix 2	o-xylene	3218.328
Set A Mix 2	1-methylethylbenzene	6.276
Set A Mix 2	1-methyl-3-ethylbenzene	2.008
Set A Mix 3	benzene-d6	2000.000
Set A Mix 3	benzene	1050.842
Set A Mix 3	ethylbenzene-d10	2000.000
Set A Mix 3	Toluene	6135.020
Set A Mix 3	ethylbenzene	1061.107