Version

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LEOSON BV

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QuantBrowser startershandbook

LEOSON BV

Product manual

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Table of Contents

Chapter 1

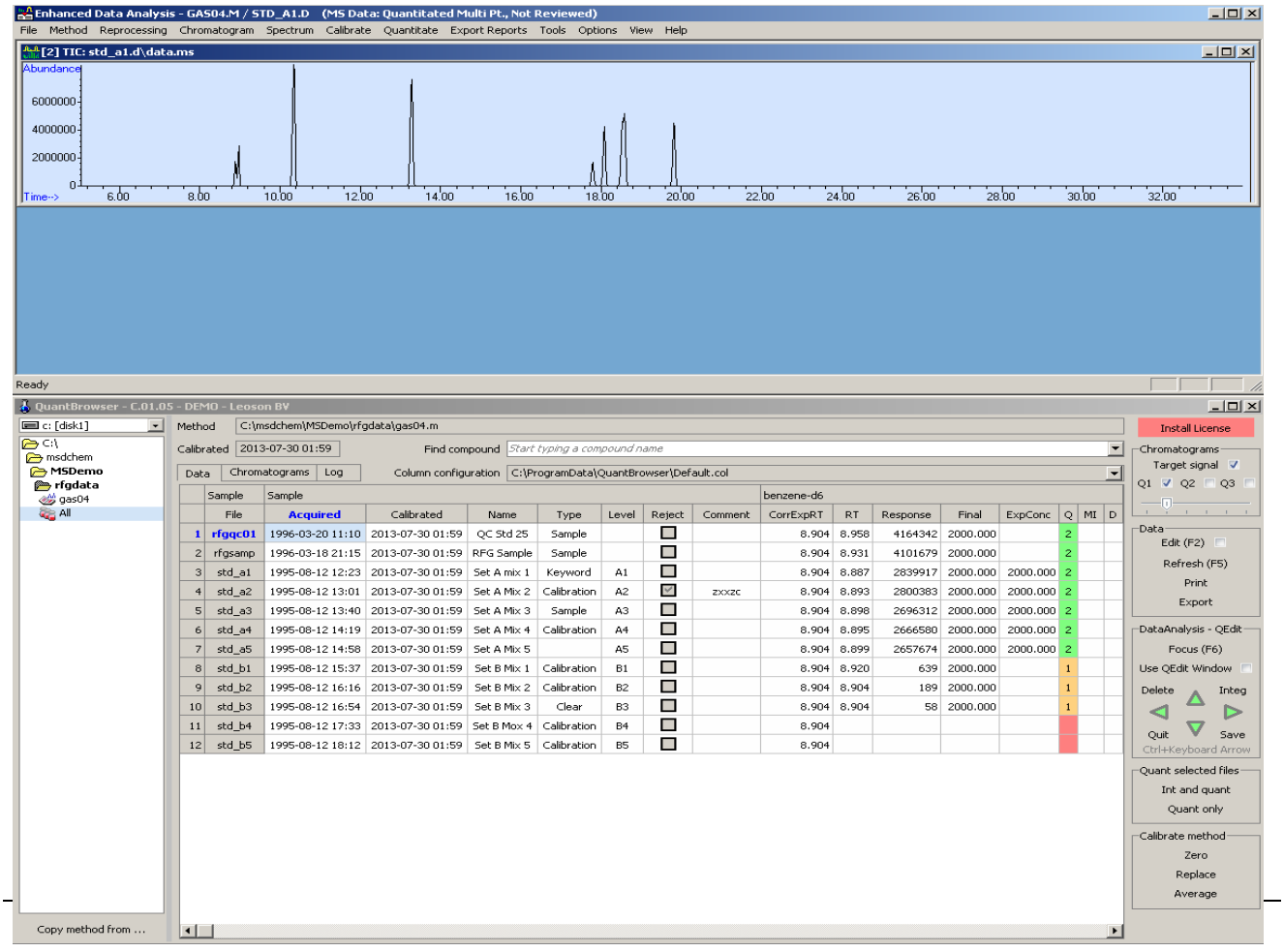
Introduction

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.

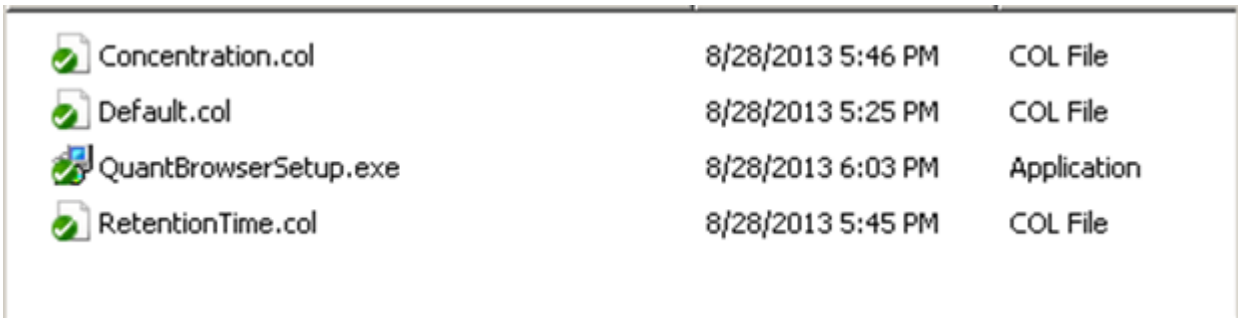


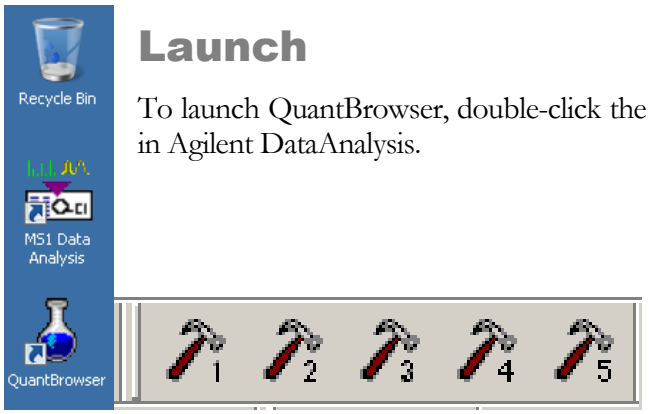
Supported platform

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).



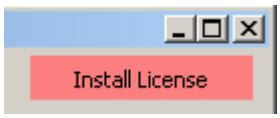


Launch

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.waleson.eu.

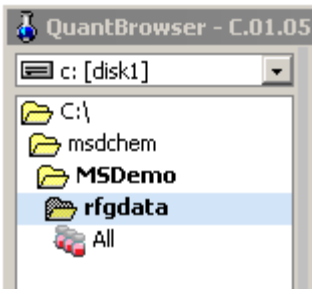


Chapter 2

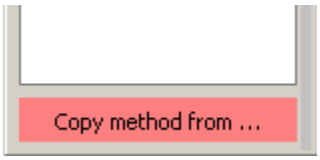
Quick Start

Prepare a dataset

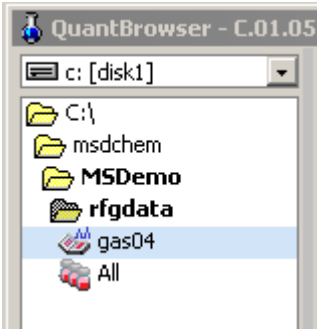
1. Navigate to the data folder



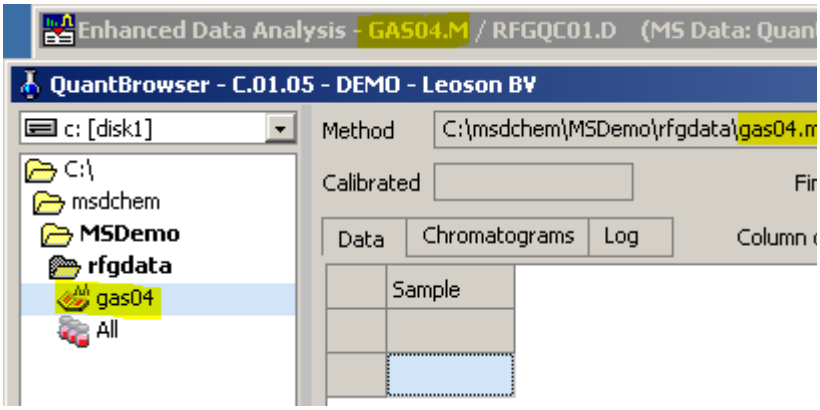
2. Copy a method to the data folder



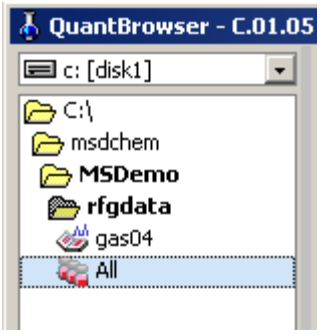
3. Load the method in DataAnalysis, double-click on the method



4. Find the loaded method name in DataAnalysis title



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

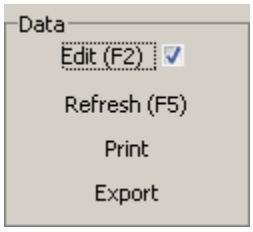


6. Find the samples and results in the table

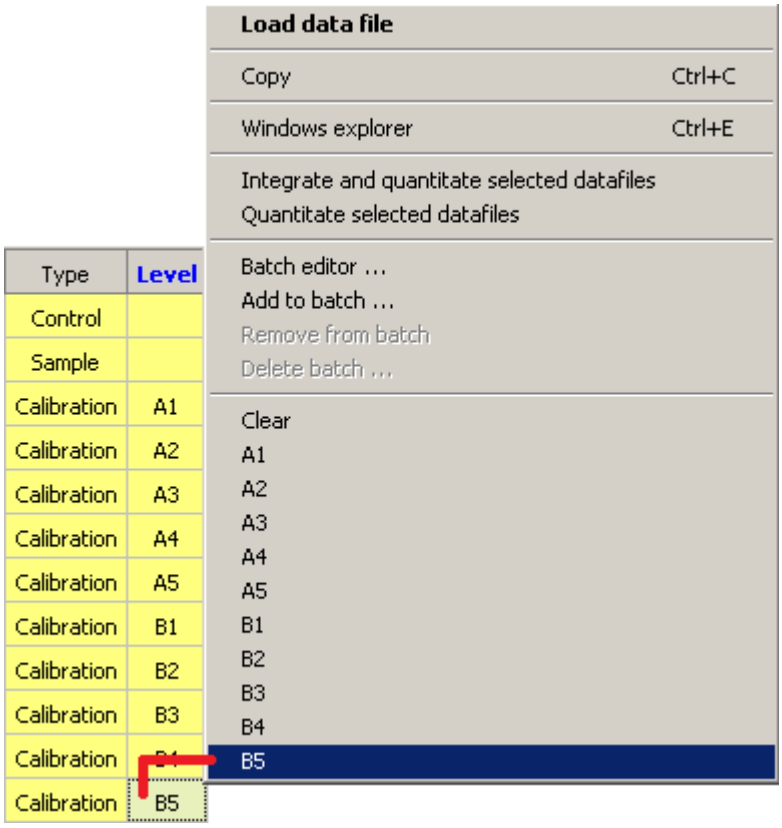
	Sample	Sample							benzene-d6						
	File	Acquired	Calibrated	Name	Type	Level	Reject	Comment	Response	Final	ExpConc	Accuracy	Q	MI	D
1	rfgqc01	1996-03-20 11:10	2013-07-30 01:59	QC Std 25			☐		4164342	2000.000			2		
2	rfgsamp	1996-03-18 21:15	2013-07-30 01:59	RFG Sample			☐		4101679	2000.000			2		
3	std_a1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

Calibrate

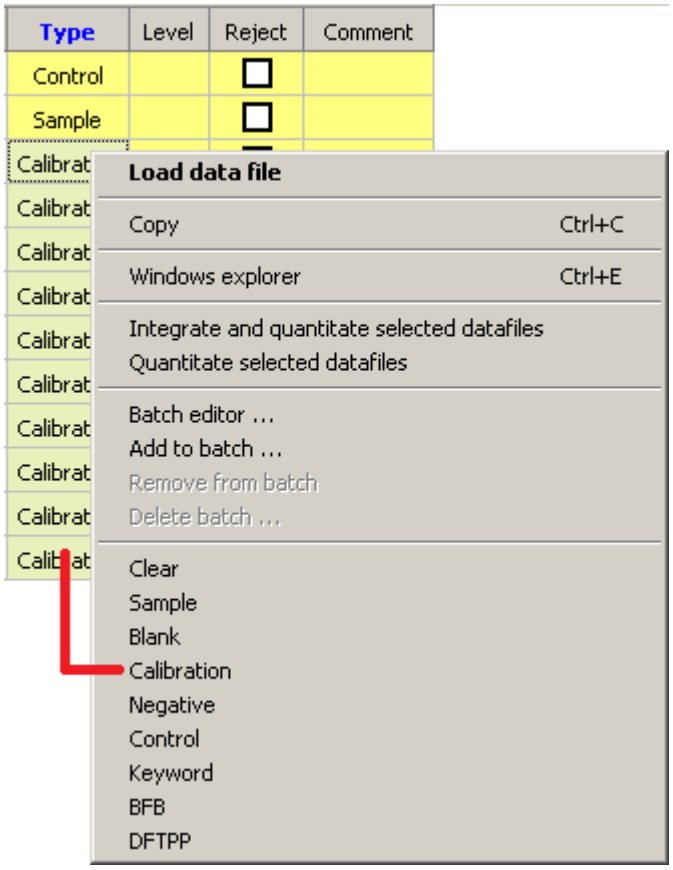
1. Edit sample type and level



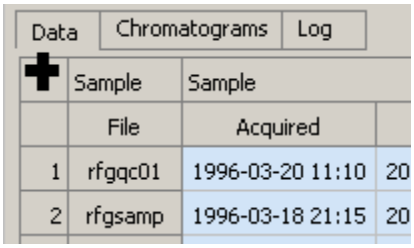
2. Set calibration levels, right click in level column



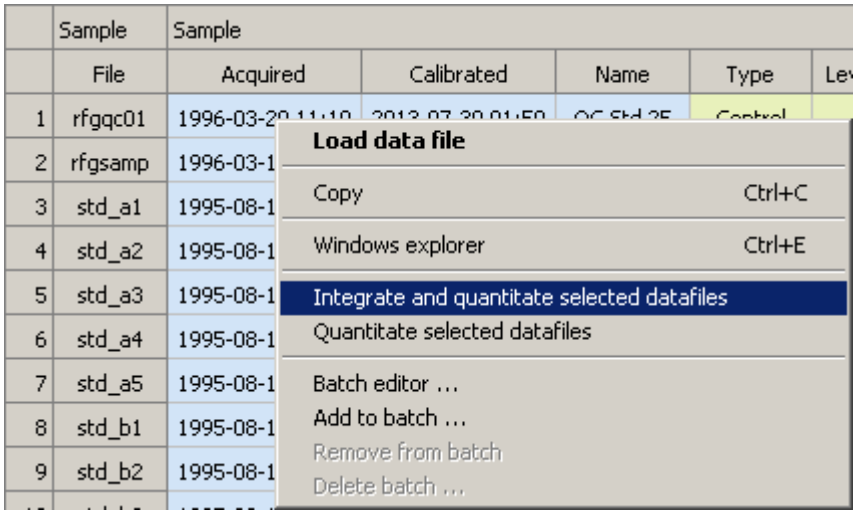
3. **Set sample type, right click in type column**



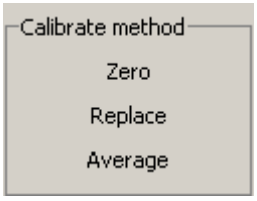
4. **Select all samples, click in upper left corner**



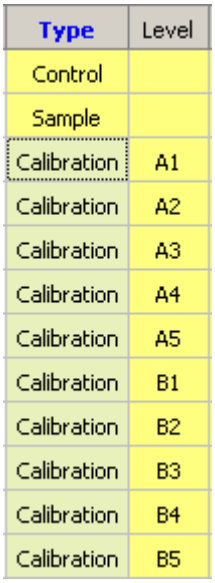
5. **Integrate and quantitate selected samples**



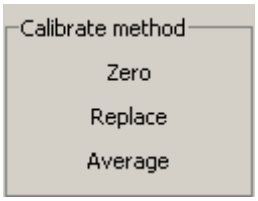
6. **Zero all responses in the calibration table, click on Zero**



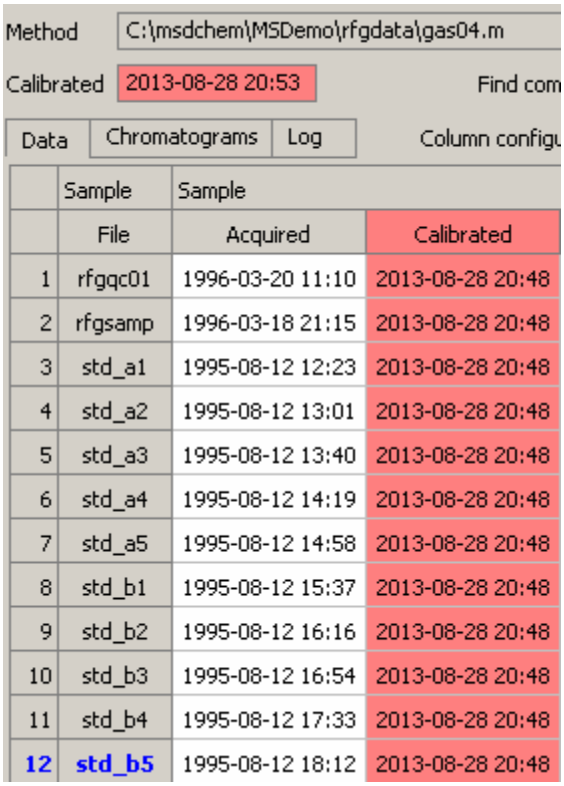
7. **Select the calibration samples**



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



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



Method C:\msdchem\MSDemo\rfgdata\gas04.m

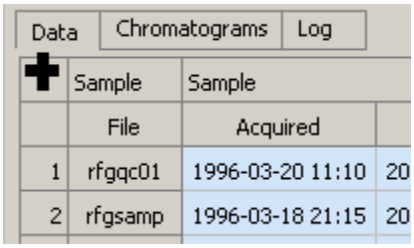
Calibrated 2013-08-28 20:53 Find com

Data | Chromatograms | Log Column configu

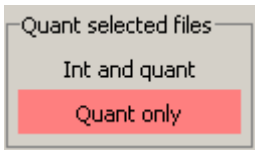
	Sample File	Sample Acquired	Sample Calibrated
1	rfgqc01	1996-03-20 11:10	2013-08-28 20:48
2	rfgsamp	1996-03-18 21:15	2013-08-28 20:48
3	std_a1	1995-08-12 12:23	2013-08-28 20:48
4	std_a2	1995-08-12 13:01	2013-08-28 20:48
5	std_a3	1995-08-12 13:40	2013-08-28 20:48
6	std_a4	1995-08-12 14:19	2013-08-28 20:48
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

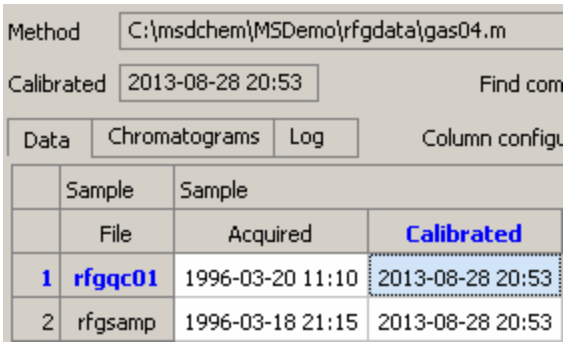
1. **Select all samples**



2. **Requantitate all samples, click on Quant only**

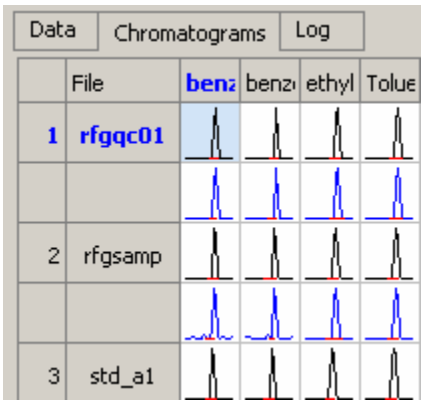


3. **Note that the samples were quantitated with the current calibration table**

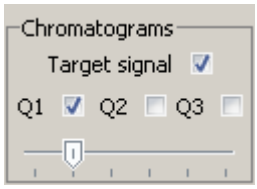


Review integration

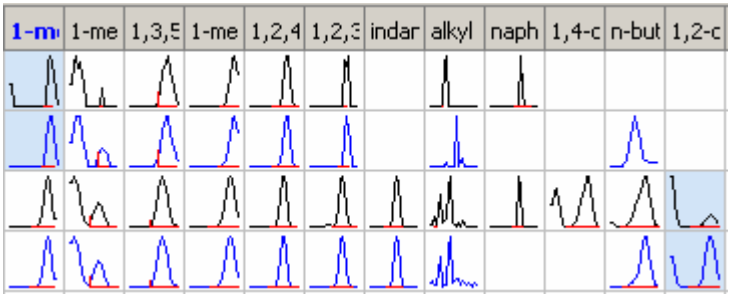
1. Review integration, click on the Chromatogram tab



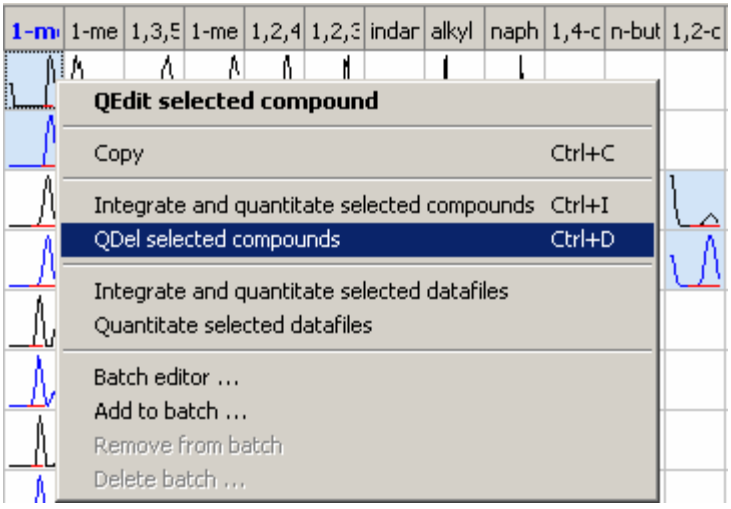
2. Select the signals and resize the plots



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



4. Delete false peaks

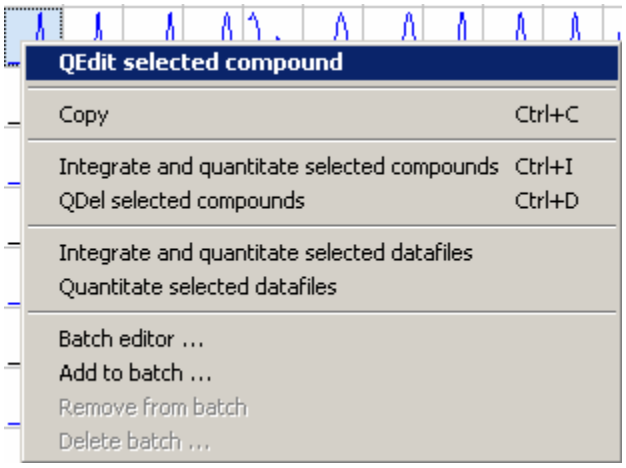


QEdit

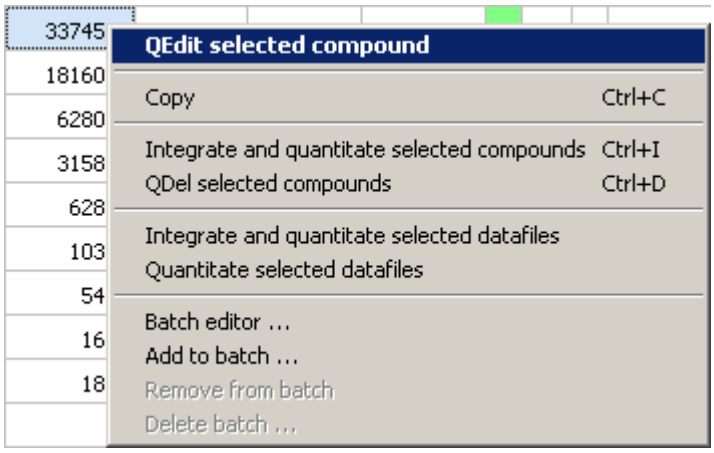
1. Note the Response and MI value for o-xylene of std_a1

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

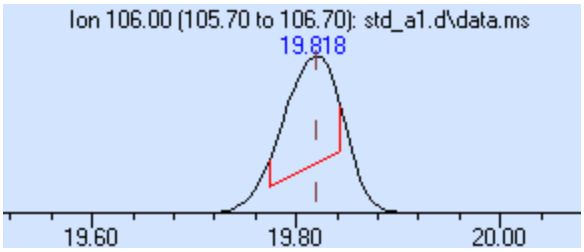


   b. QEdit from Data tab, right click menu, or double click on a compound cell

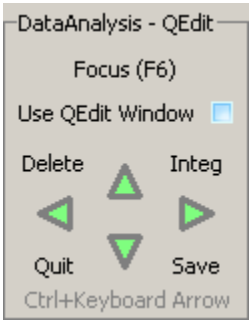


   c. QEdit with navigation arrow

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**

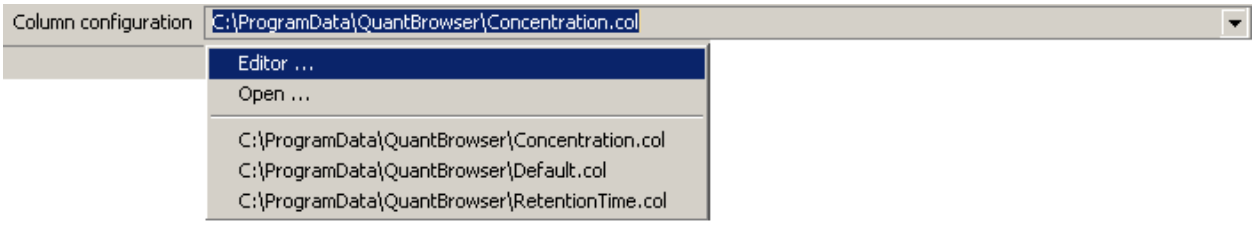


5. **Note the new values for o-xylene of std_a1.**

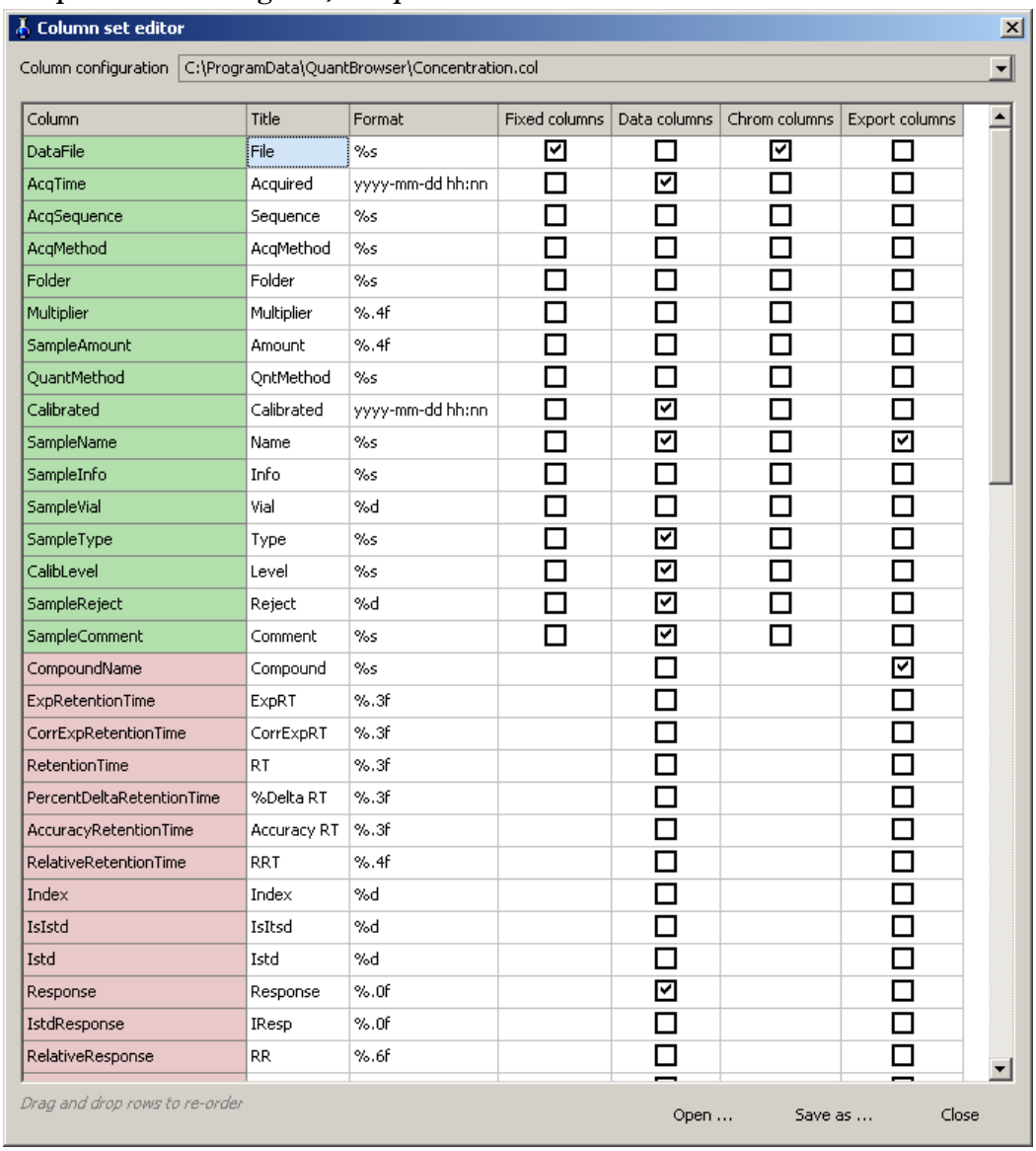
o-xylene						
Response	Final	ExpConc	Accuracy	Q	MI	D
2155357	2327.603			2		
2078636	2111.687			2		
1738070	3023.957	6000.000	50.40	1	1	
1816025	3218.328	3000.000	107.28	2		

Column configuration

1. **New column configurations can be created**



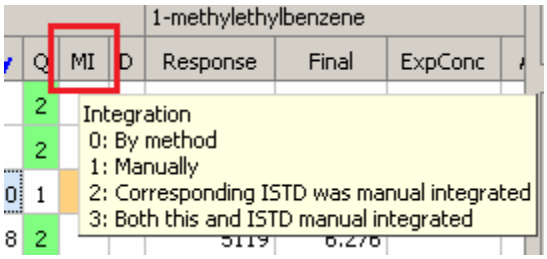
2. **Column can be selected and re-order by drag and drop.**
   Sample columns are green, compound columns are red.



Column	Title	Format	Fixed columns	Data columns	Chrom columns	Export columns
DataFile	File	%s	☑	☐	☑	☐
AcqTime	Acquired	yyyy-mm-dd hh:nn	☐	☑	☐	☐
AcqSequence	Sequence	%s	☐	☐	☐	☐
AcqMethod	AcqMethod	%s	☐	☐	☐	☐
Folder	Folder	%s	☐	☐	☐	☐
Multiplier	Multiplier	%.4f	☐	☐	☐	☐
SampleAmount	Amount	%.4f	☐	☐	☐	☐
QuantMethod	QntMethod	%s	☐	☐	☐	☐
Calibrated	Calibrated	yyyy-mm-dd hh:nn	☐	☑	☐	☐
SampleName	Name	%s	☐	☑	☐	☑
SampleInfo	Info	%s	☐	☐	☐	☐
SampleVial	Vial	%d	☐	☐	☐	☐
SampleType	Type	%s	☐	☑	☐	☐
CalibLevel	Level	%s	☐	☑	☐	☐
SampleReject	Reject	%d	☐	☑	☐	☐
SampleComment	Comment	%s	☐	☑	☐	☐
CompoundName	Compound	%s		☐		☑
ExpRetentionTime	ExpRT	%.3f		☐		☐
CorrExpRetentionTime	CorrExpRT	%.3f		☐		☐
RetentionTime	RT	%.3f		☐		☐
PercentDeltaRetentionTime	%Delta RT	%.3f		☐		☐
AccuracyRetentionTime	Accuracy RT	%.3f		☐		☐
RelativeRetentionTime	RRT	%.4f		☐		☐
Index	Index	%d		☐		☐
IsIstd	IsItsd	%d		☐		☐
Istd	Istd	%d		☐		☐
Response	Response	%.0f		☑		☐
IstdResponse	IResp	%.0f		☐		☐
RelativeResponse	RR	%.6f		☐		☐

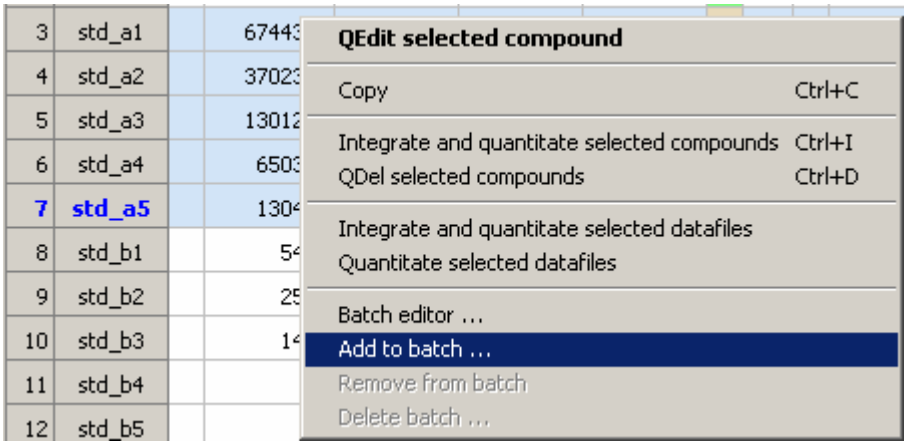
Column information

1. Rest the mouse above a column header

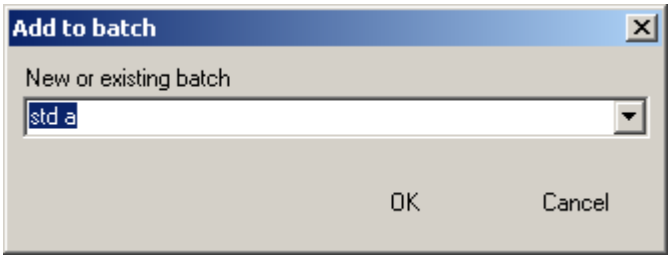


Sample batch

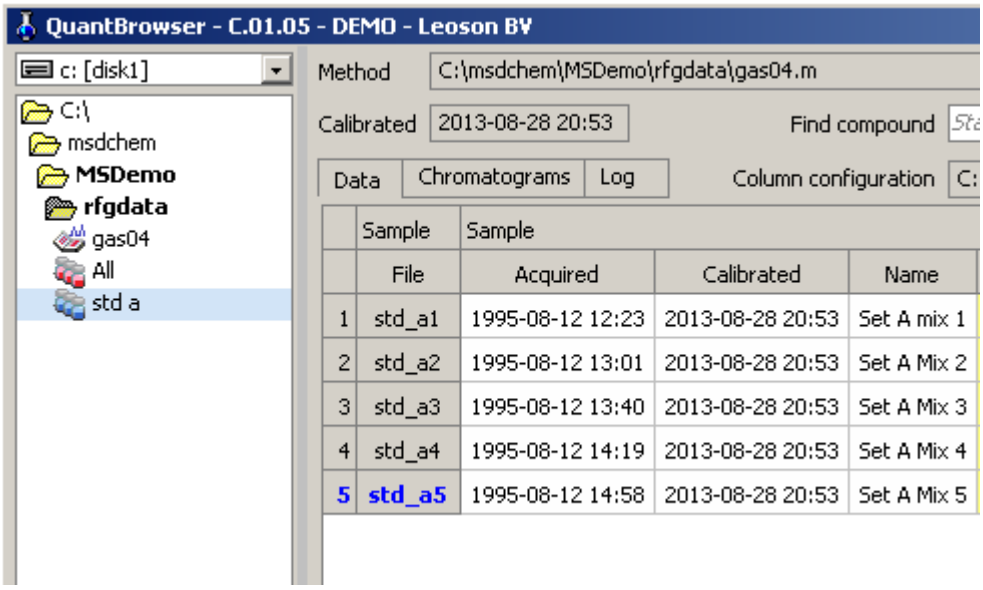
1. Select sample for the batch, right click on the samples and Add to batch



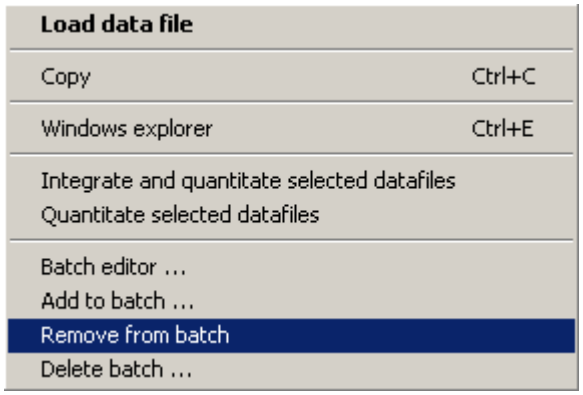
2. Specify the batch name



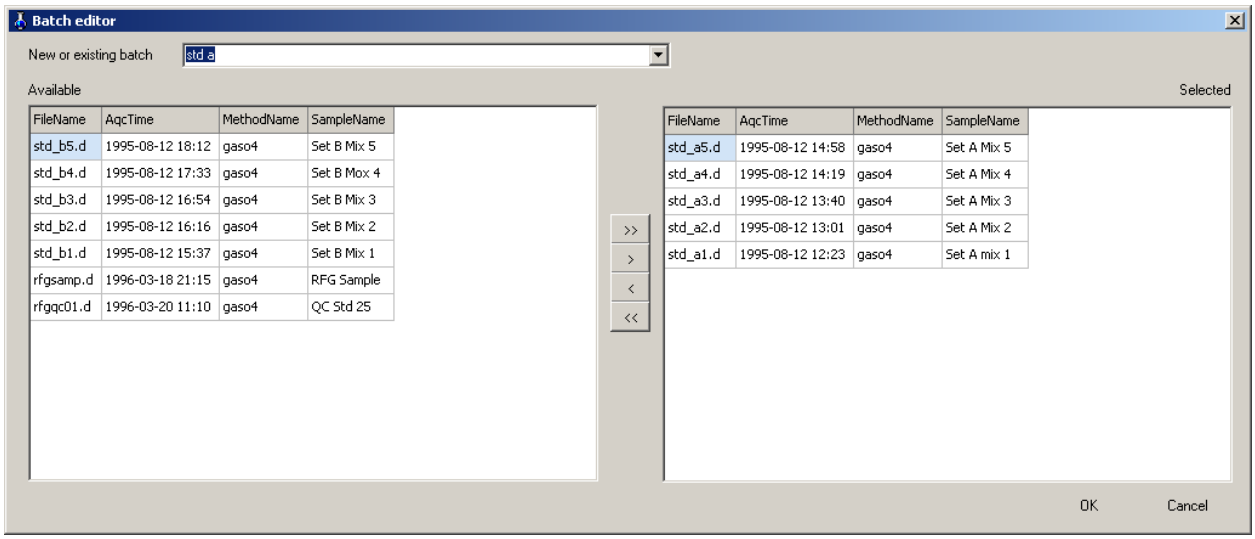
3. Find the samples in the new batch



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**

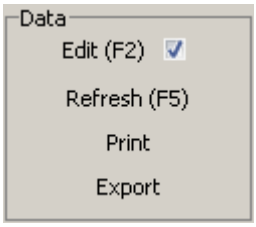


Copy to clipboard

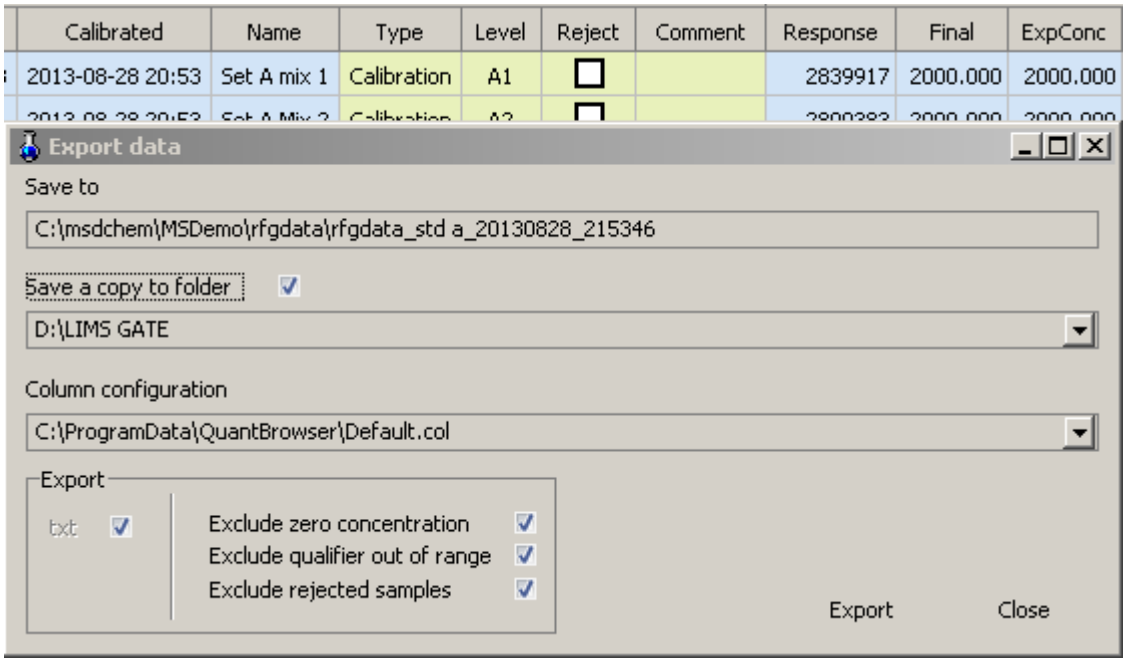
1. **Select table cells and copy to clipboard. Use the right click menu in the table.**

Export data

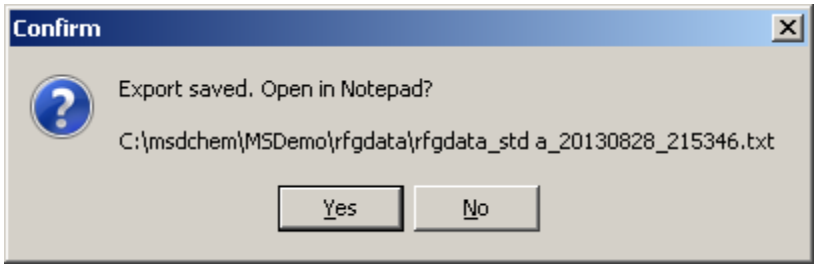
1. **Open the export dialog, click on export button**



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



3. **Open the results in Notepad**



4. View the results