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Quant Browser

for the
Agilent Technologies GCMS Chemstation

Main purposes of Quant Browser

- Improve productivity of the quantitation process.
- Collect quantitation results of a complete sequence in a single sheet.
- Give easy access to QEdit and update automatically after manual integration.
- Export results to Excel and optional to a LIMS system.
- Generate optional High Density Quant Reports to review and archive peak integration baselines.

Content

Supported Platform

Quant Browser is supported on the following GCMS Chemstation versions.

G1701BA B.00.01	Tested
G1701CA C.00.01	Tested
G1701DA D.00.00	Tested
G1701DA D.01.00	Tested
G1701DA D.02.00	Tested
G1701DA D.03.00	Tested
G1701EA E.01.00	Tested

Installation

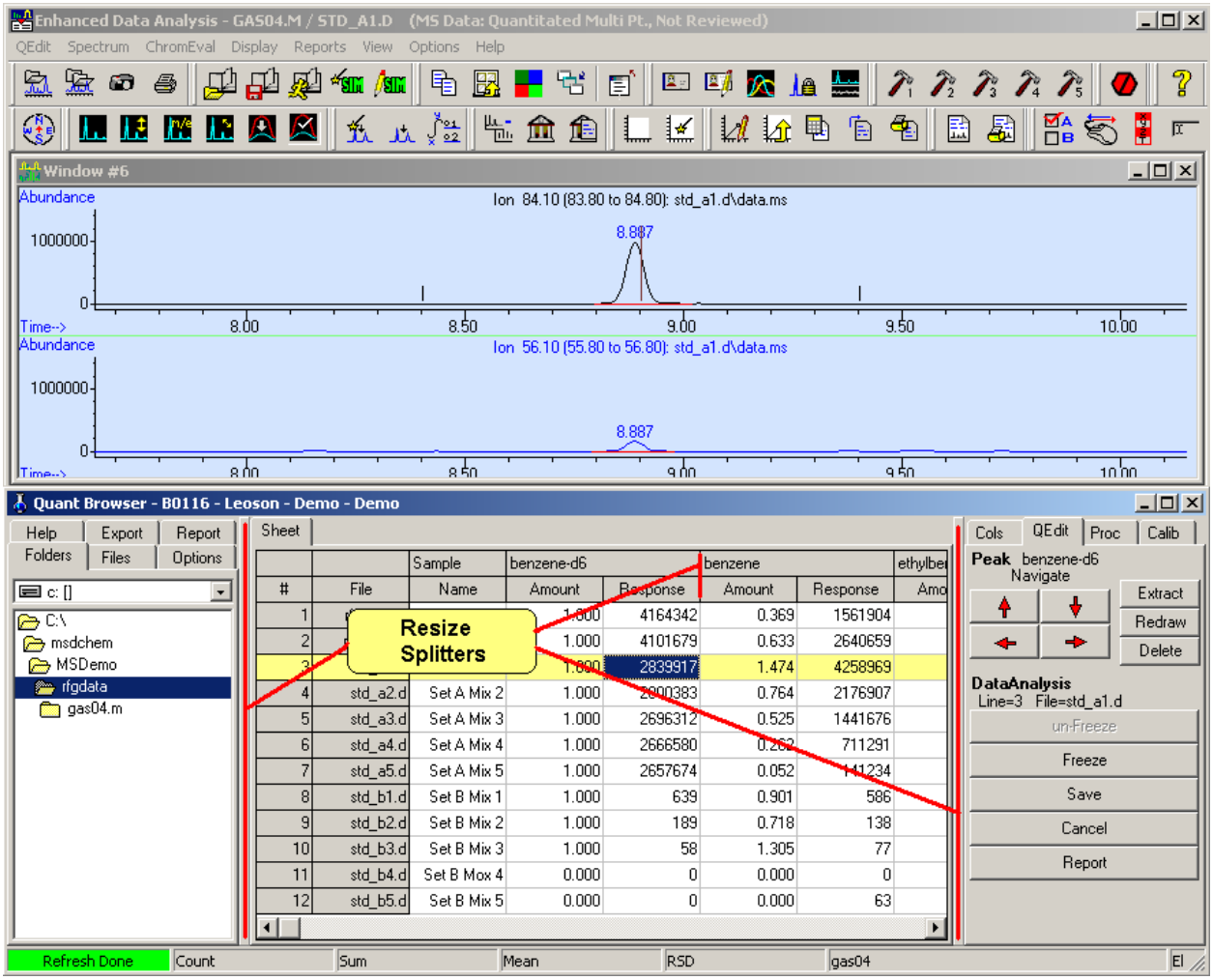
Quant Browser is distributed as a single file installer program. The installer will check whether the supported (GCMS) Chemstation is installed. However , the version of the Chemstation is not checked. After execution of the installer, a dialog should appear with the new version number and the old version number of the eventual currently installed program.

After installation, Quant Browser can be started by a icon on the desktop.

De-installation should be done with the same installer program. There is no entry in the Windows Add-Remove Programs list.

After de-installation, certain methods might still contain the Method-Automation entry in the Custom Analysis macro. This is only after one used the Method-Automation option button (page 8).

The Result Sheet



#	File	Sample Name	benzene-d6 Amount	benzene-d6 Response	benzene Amount	benzene Response	ethylbe Amo
1			1.000	4164342	0.369	1561904	
2			1.000	4101679	0.633	2640659	
3			1.000	2839917	1.474	4258969	
4	std_a2.d	Set A Mix 2	1.000	2900383	0.764	2176907	
5	std_a3.d	Set A Mix 3	1.000	2696312	0.525	1441676	
6	std_a4.d	Set A Mix 4	1.000	2666580	0.267	711291	
7	std_a5.d	Set A Mix 5	1.000	2657674	0.052	141234	
8	std_b1.d	Set B Mix 1	1.000	639	0.901	586	
9	std_b2.d	Set B Mix 2	1.000	189	0.718	138	
10	std_b3.d	Set B Mix 3	1.000	58	1.305	77	
11	std_b4.d	Set B Mox 4	0.000	0	0.000	0	
12	std_b5.d	Set B Mix 5	0.000	0	0.000	63	

The sheet contains
-sample information
-compound quantitation results
There are many columns available. Only selected columns are displayed.

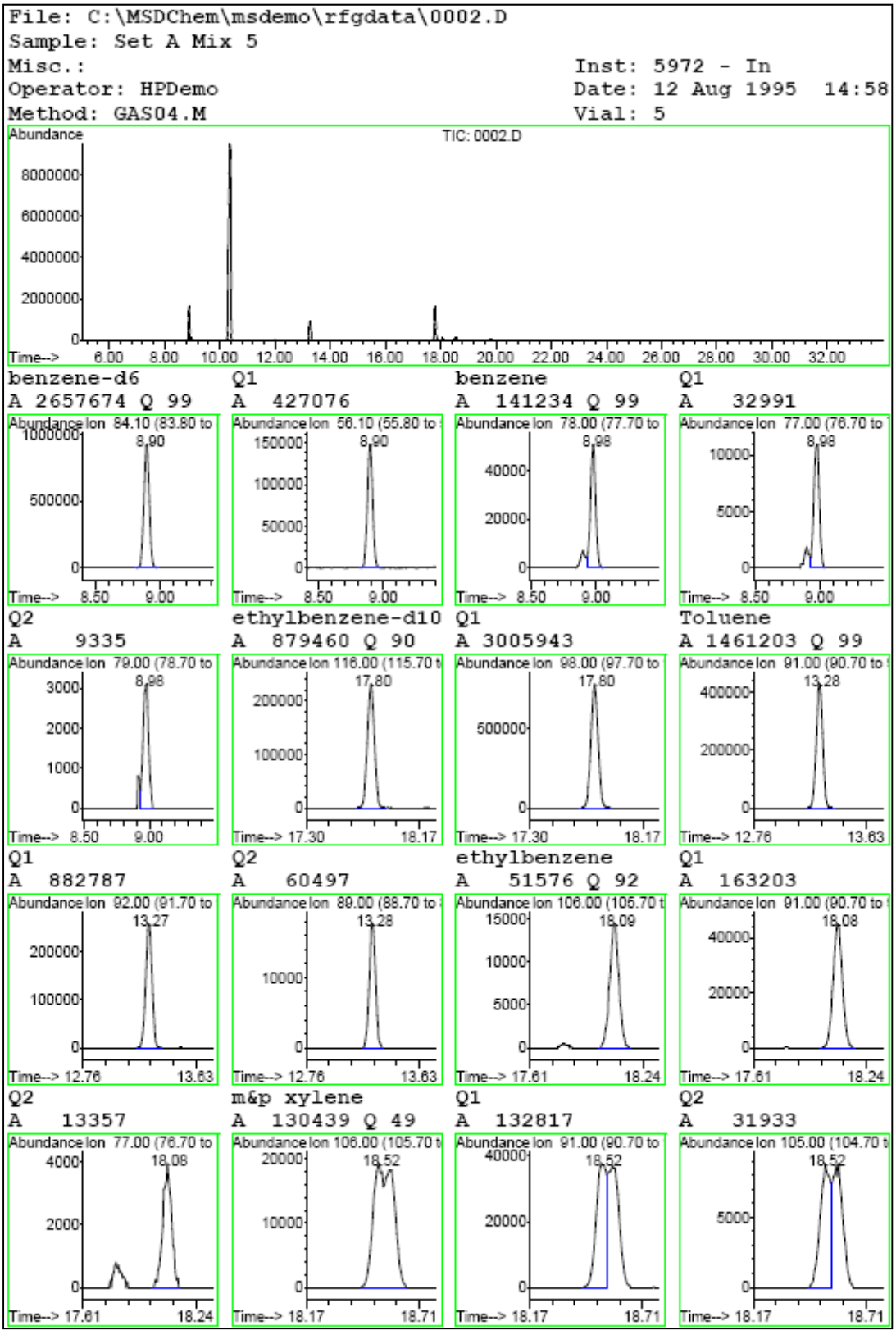
Values are constantly imported from each data file when required.

Double click on a compound value opens the QEdit tab and displays the peak integration in Data Analysis (picture). A manual integration can be performed in Data Analysis. Navigation to another value or row will save the manual integration and update the sheet in real-time. Navigation can be done by double click in the sheet, the red arrow buttons or the cursor keys on the keyboard.

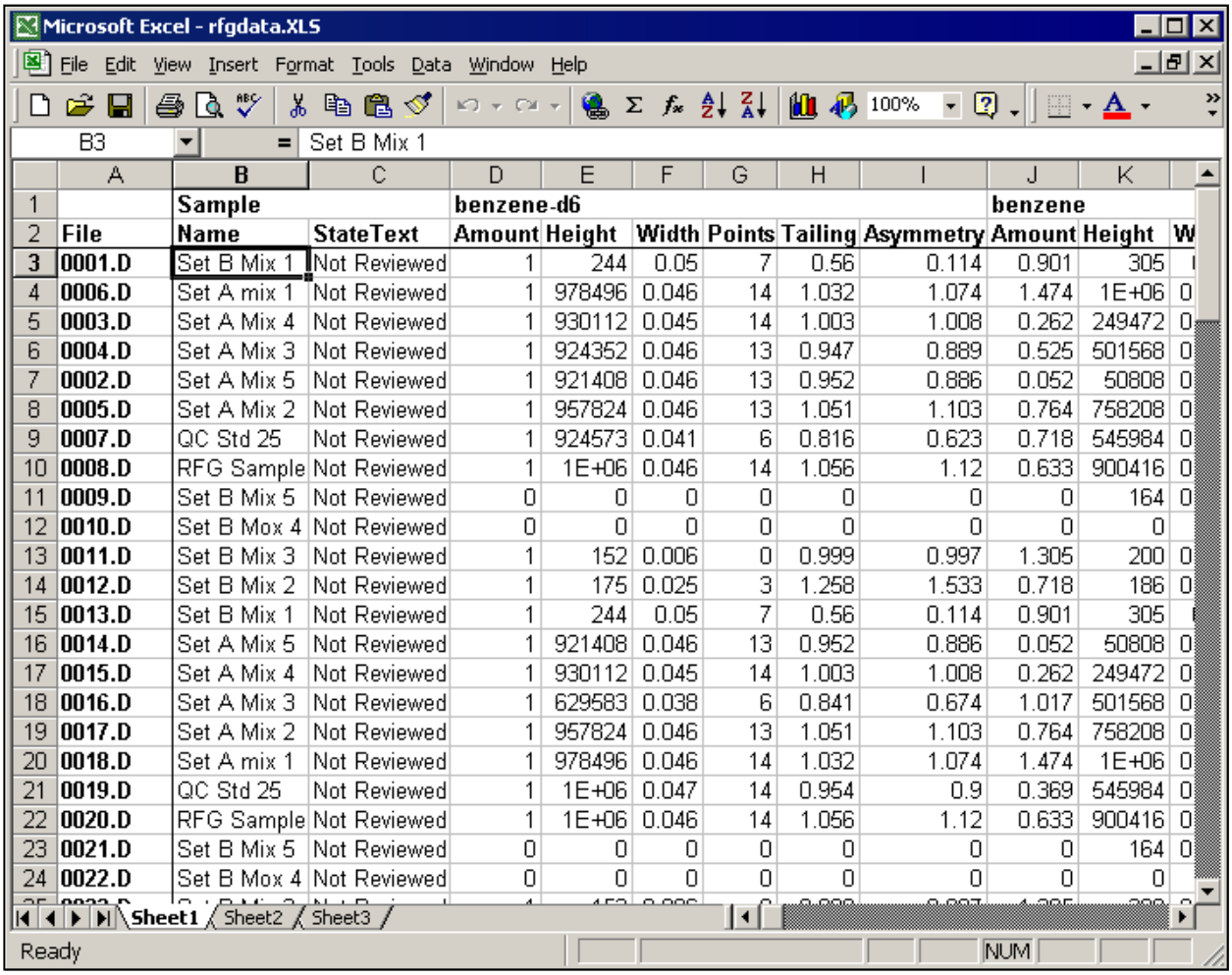
Click on a data file (second column) will load the data file in DataAnalysis
Click on first row will select the column underneath
Click on the second row will perform sorting
Column width can be adjusted by dragging the line between the columns on the second row

The left pane and right pane can be re-sized or hidden by dragging or clicking the splitter bar that separates the panes from the sheet.

Optional High Density Quant Report



Exporting to Excel



Microsoft Excel - rfgdata.XLS

File Edit View Insert Format Tools Data Window Help

B3 = Set B Mix 1

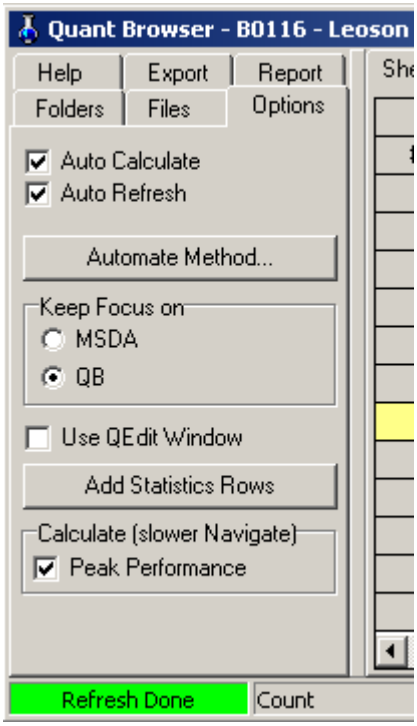
	A	B	C	D	E	F	G	H	I	J	K	
1		Sample		benzene-d6						benzene		
2	File	Name	StateText	Amount	Height	Width	Points	Tailing	Asymmetry	Amount	Height	W
3	0001.D	Set B Mix 1	Not Reviewed	1	244	0.05	7	0.56	0.114	0.901	305	
4	0006.D	Set A mix 1	Not Reviewed	1	978496	0.046	14	1.032	1.074	1.474	1E+06	0
5	0003.D	Set A Mix 4	Not Reviewed	1	930112	0.045	14	1.003	1.008	0.262	249472	0
6	0004.D	Set A Mix 3	Not Reviewed	1	924352	0.046	13	0.947	0.889	0.525	501568	0
7	0002.D	Set A Mix 5	Not Reviewed	1	921408	0.046	13	0.952	0.886	0.052	50808	0
8	0005.D	Set A Mix 2	Not Reviewed	1	957824	0.046	13	1.051	1.103	0.764	758208	0
9	0007.D	QC Std 25	Not Reviewed	1	924573	0.041	6	0.816	0.623	0.718	545984	0
10	0008.D	RFG Sample	Not Reviewed	1	1E+06	0.046	14	1.056	1.12	0.633	900416	0
11	0009.D	Set B Mix 5	Not Reviewed	0	0	0	0	0	0	0	164	0
12	0010.D	Set B Mox 4	Not Reviewed	0	0	0	0	0	0	0	0	
13	0011.D	Set B Mix 3	Not Reviewed	1	152	0.006	0	0.999	0.997	1.305	200	0
14	0012.D	Set B Mix 2	Not Reviewed	1	175	0.025	3	1.258	1.533	0.718	186	0
15	0013.D	Set B Mix 1	Not Reviewed	1	244	0.05	7	0.56	0.114	0.901	305	
16	0014.D	Set A Mix 5	Not Reviewed	1	921408	0.046	13	0.952	0.886	0.052	50808	0
17	0015.D	Set A Mix 4	Not Reviewed	1	930112	0.045	14	1.003	1.008	0.262	249472	0
18	0016.D	Set A Mix 3	Not Reviewed	1	629583	0.038	6	0.841	0.674	1.017	501568	0
19	0017.D	Set A Mix 2	Not Reviewed	1	957824	0.046	13	1.051	1.103	0.764	758208	0
20	0018.D	Set A mix 1	Not Reviewed	1	978496	0.046	14	1.032	1.074	1.474	1E+06	0
21	0019.D	QC Std 25	Not Reviewed	1	1E+06	0.047	14	0.954	0.9	0.369	545984	0
22	0020.D	RFG Sample	Not Reviewed	1	1E+06	0.046	14	1.056	1.12	0.633	900416	0
23	0021.D	Set B Mix 5	Not Reviewed	0	0	0	0	0	0	0	164	0
24	0022.D	Set B Mox 4	Not Reviewed	0	0	0	0	0	0	0	0	

Sheet1 Sheet2 Sheet3

Ready NUM

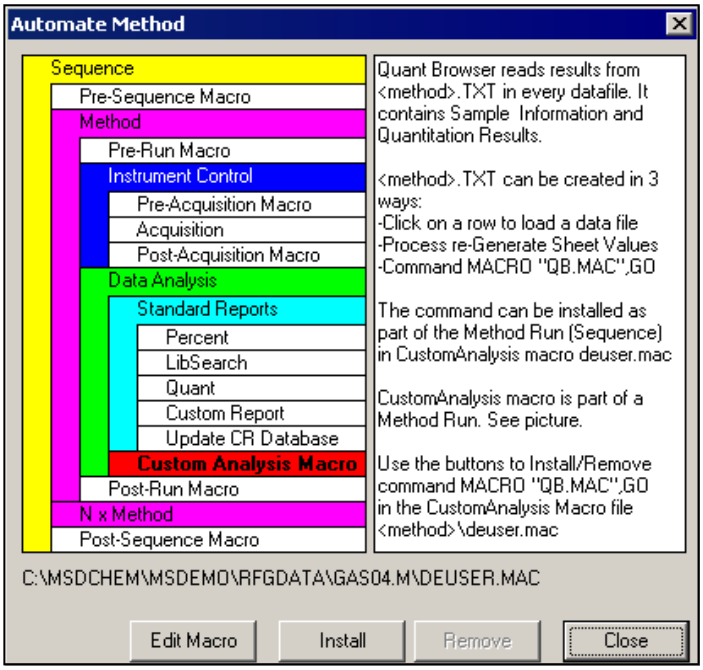
The native XLS file export ensures correct transfer of the decimal separator and date-time values, regardless of the language or regional settings on the computer. The export is limited by Excel to 256 columns.

Options



Auto Calculate	Navigate to a new folder will load the result for the current method. If the data files do not have result for the current method, a dialog will ask for automatic recalculations.
Auto Refresh	Quant Browser monitors the selected data folder. New files and new values are detected and displayed
Automate Method...	Sheet values are stored in each data file. For convenience they can already be generated during a sequence.
Keep Focus on MSDA	Double click on a sheet value will load the compound in Data Analysis and activates the Data Analysis window
Keep Focus on QB	Successive navigation with keyboard cursor keys will be possible when the Quant Browser window stays activated
Use QEdit Window	All compounds are accessible in the sheet and therefore the Chemstation QEdit window is not required
Add Statistics Rows	Statistics rows can be display temporarily at the bottom of the sheet
Peak Performance	Values like Height, Width, Asymmetry, Tailing and Points will slow down navigation a little.

Method Automation

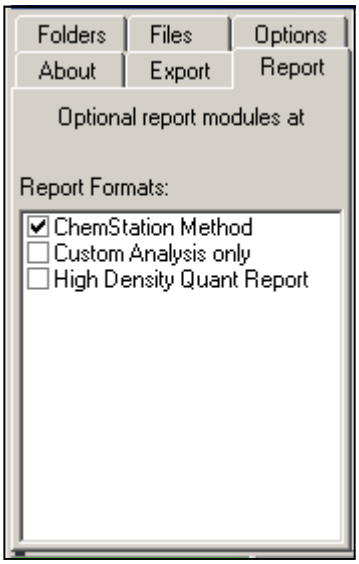


Method Automation is useful during a acquisition sequence on the Instrument PC, or when sequence reprocessing is used on an Offline PC. This will pre-generate the sheet values in each data file. The method in the sequence must have the same name as the method used with Quant Browser.

The Method Automation will only save little time. Typically Quant Browser re-generates sheet values within 1s per data file.

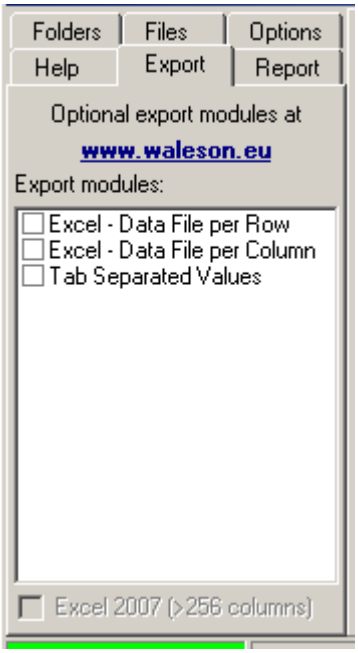
The Method Automation will still be useful though. It stores sequence information that would be lost otherwise: see page 11.

Report Modules



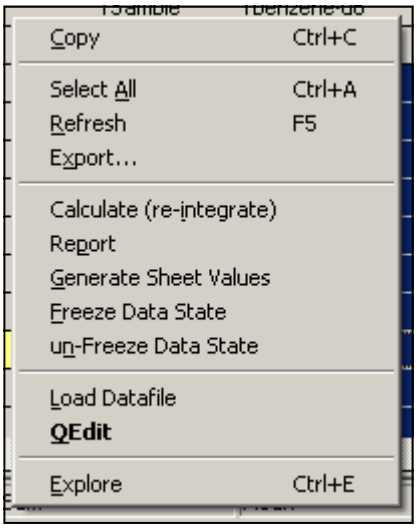
ChemStation Method	The reports as specified in the Method. This includes the Custom Analysis macro.
Custom Analysis only	Executes the <method>\user.mac macro
High Density Quant Report	Optional. Useful for reviewing or archiving the integrated baselines. Save printed pages.
Optional Report Modules	Option Modules can be obtained from the vendor

Export Modules



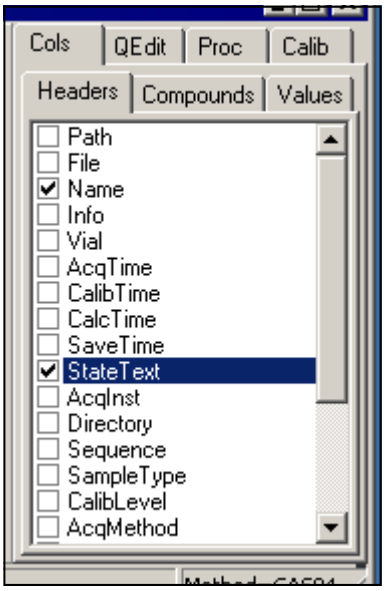
Excel	The native XLS file export ensures correct transfer of the decimal separator and date-time values, regardless of the language or regional settings on the computer. The export is limited by Excel to 256 columns.
Tab Separated Values	Exports sheet values with unlimited selected number of columns. The decimal separator is the US English dot like in the Chemstation.
Optional Export Modules	Option Modules can be obtained from the vendor

Right Click Sheet Menu



Copy	Copy selected cells to Clipboard
Select All	Select all cells
Refresh	Clears the sheet and read all the values again
Export	Export by using the selected Export Module
Calculate	Re-Integrated and quantitate all not-Frozen data files
Report	Report by using the selected Report Module
Generate Sheet Values	Load each selected data file and save the sheet values in each data file. Quant Browser will automatically read all new generated values.
Freeze Data State	The integration baselines of a Frozen data file can not be overwritten by the used method. Different methods can be used to integrate a data file. Each method has it own integration result file stored in the data file. Each can be frozen independently.
Un-Freeze Data State	The data file can be re-integrated again.
Load Data file	Just load the data file. The same can be achieved by a click on a cell in the file name column.
QEdit	Opens QEdit for manual integration on the selected compound. The same can be achieved by clicking on any cell in a compound column.
Explore	Open the data file folder in Windows Explorer

Header Columns

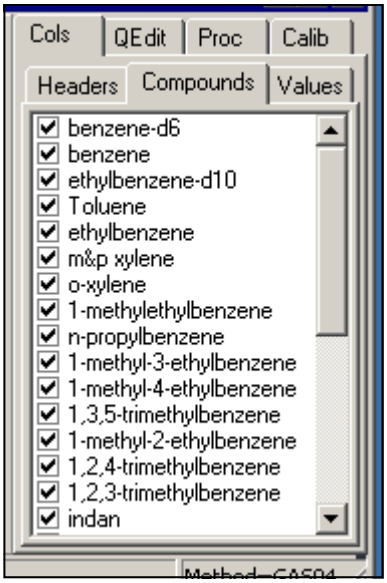


Path	Path where the data file can be found
File	The .D file name
Name	Sample Name (14 characters)
Info	Sample Info (14 characters)
Vial	Vial number
Multiplier	Sample Multiplier (not for ISTD)
Amount	Sample Amount (not for ISTD)
AcqTime	Acquisition Time
CalibTime	Calibration Time of the method
CalcTime	Integration and Quantitation Time
SaveTime	Saving of sheet values Time
StateText	Not-Reviewed or Frozen
AcqInst	Acquisition Instrument
Directory	Directory where the data file can be found
AcqMethod	Acquisition Method (19 characters)
CalcMethod	Calculation Method
SaveMethod	Save of sheet values Method
ActBarcode	Actual Barcode
ExpBarcode	Expeced Barcode
Operator	Operator

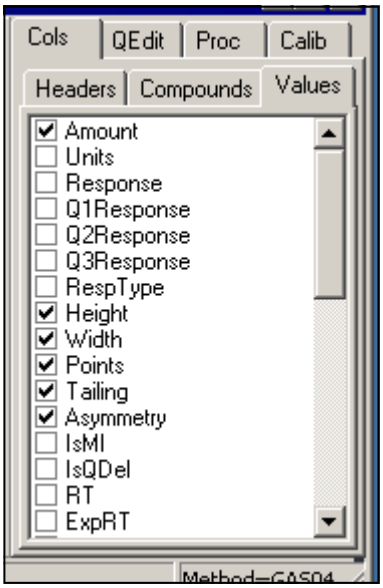
Only when Method Automation was used during Acquisition:

Sequence	Sequence File
SampleType	Blank, Sample, Calibration
CalibLevel	Calibration Level
SeqIndex	Sequence Line
Replicate	Injection per Vial
SeqMethod	Sequence Method (>19 characters)

Compound Columns

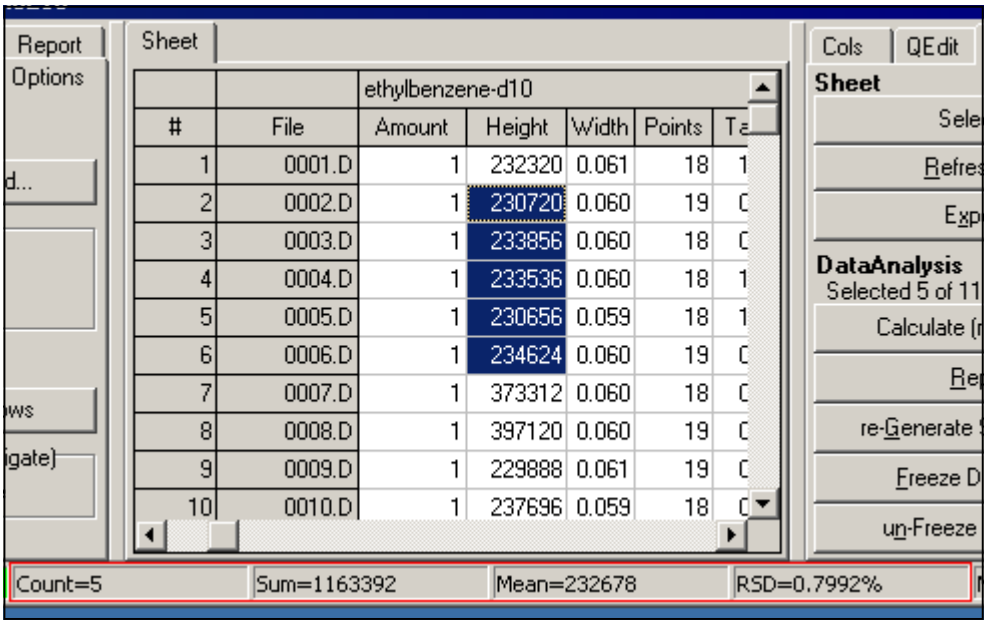


Values Columns



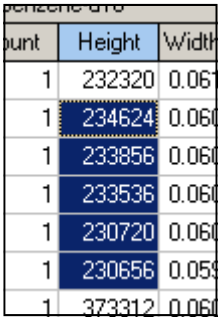
Name	Compound Name
Amount	Amount
Units	Amount Units
AmountRaw	Amount without Sample Amount and Multiplier
ExpAmount	Expected compound Amount. Useful for control samples. Extracted for each non-ISTD from the SampeName. The values should be between dashes '-' and separated by pipes '|'. Example: Sample A -1.1|2.2|3.3-
Accuracy	100-(ExpAmount-MultAmount)/ExpAmount*100
Response	Response as Area or Height depending on the selection in the Calibration table.
RespRatio	Response/ISTD Response
Q1Response	Qualifier 1 Response
Q2Response	Qualifier 2 Response
Q3Response	Qualifier 3 Response
RespType	Keyword: Area or Height
Height	Target Peak Height
Width	Target Peak Width
Points	Target Peak width in Data Points (At 5% Height)
Tailing	Target Peak Tailing according to USP: (TEnd-TStart)/2/ (RT-TStart) at 5% height
Asymmetry	Target Peak Asymmetry according to IUPAC and ASTM: (TEnd-RT)/(RT-TStart) at 10% height
IsMI	Is any of the compound peaks manual integrated
IsQDel	Is the compound 'deleted'
RT	Retention Time in minutes
ExpRT	Expected Retention Time in minutes
QValue	QValue by normal Chemstation Quantitation
QValueMI	QValue after Manual Integration
Ion	Target Ion
Index	Calibration Table Compound Index
IsFound	Compound Found. 0=No Peak, 1=Matched RT, 2=Matched RT and Matched Qualifiers.
IsTimeRef	Is Compound a Time Reference
IsIstd	Is Compound an Internal Standard
IstdAmount	Internal Standard Amount
IstdResponse	Internal Standard Response
IsUAbs	Qualifier Uncertainty. 0=Relative, 1=Absolute
Q1PM	Qualifier 1 Percentage Measured
Q1P	Qualifier 1 Percentage Expected
Q1UM	Qualifier 1 Uncertainty Measured
Q1U	Qualifier 1 Uncertainty Allowed
Q2PM	Qualifier 2 Percentage Measured
Q2P	Qualifier 2 Percentage Expected
Q2UM	Qualifier 2 Uncertainty Measured
Q2U	Qualifier 2 Uncertainty Allowed
Q3PM	Qualifier 3 Percentage Measured
Q3P	Qualifier 3 Percentage Expected
Q3UM	Qualifier 3 Uncertainty Measured
Q3U	Qualifier 3 Uncertainty Allowed

Selection Statistics



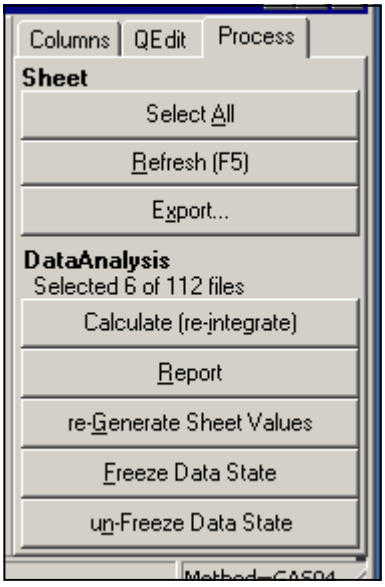
Selecting a group of cells will calculate Count, Sum, Mean and RSD% in the status bar.

Selection Sorting



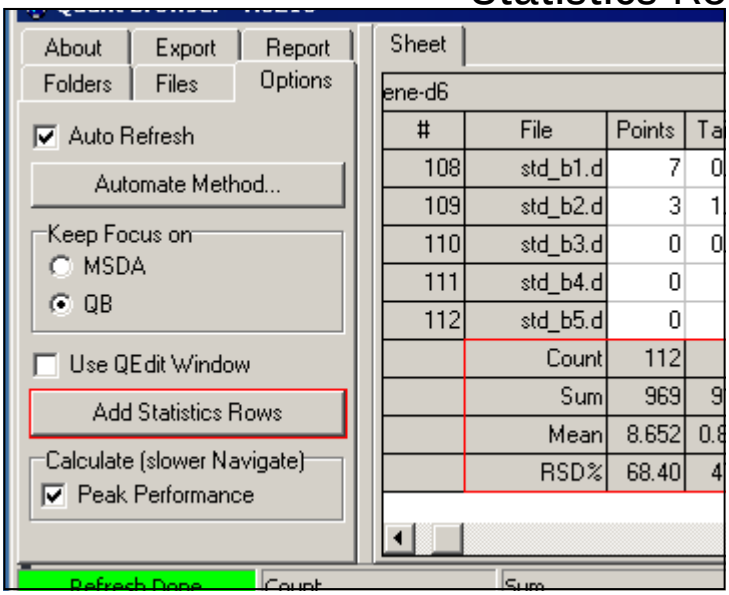
Sorting can be performed by a mouse click on the second row. If cells on only a few rows are selected, only those rows will be sorted.

Process Buttons



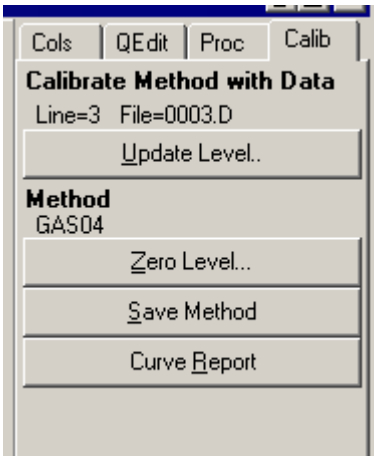
Select All	Select all cells
Refresh	Clears the sheet and read all the values again
Export	Export by using the selected Export Module
Calculate (re-Integrate)	Re-Integrated and quantitate all not-Frozen data files
Report	Report by using the selected Report Module
re-Generate Sheet Values	Load each selected data file and save the sheet values in each data file. Quant Browser will automatically read all new generated values.
Freeze Data State	The integration baselines of a Frozen data file can not be overwritten by the used method. Different methods can be used to integrate a data file. Each method has it own integration result file stored in the data file. Each can be frozen independently.
un-Freeze Data State	The data file can be re-integrated again.

Statistics Rows



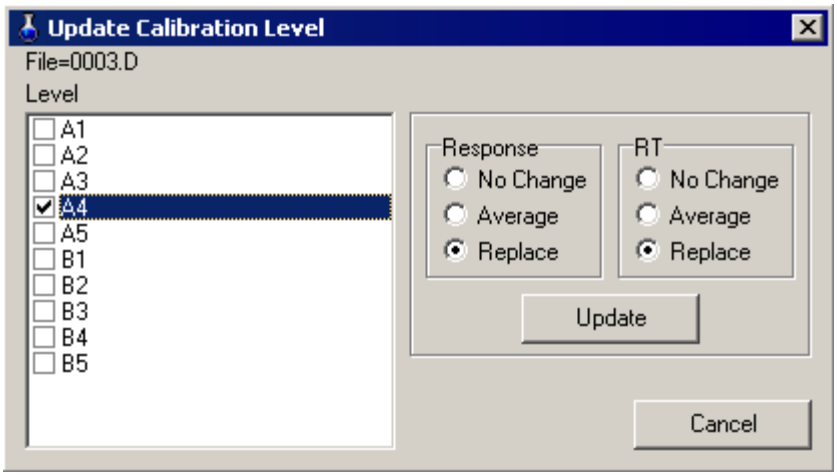
Add Statistics Rows will add four rows at the bottom of the sheet: Count, Sum, Mean, RSD%
Only numeric values will be considered in the statistics calculations.

Calibrate Buttons



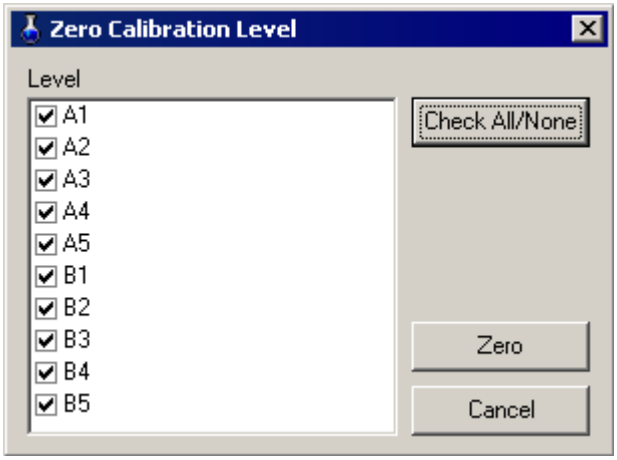
Update Level	Show dialog to update a single level of the calibration table with the current data file responses
Zero Level	Show a dialog to clear the responses of one or more levels in the calibration table
Save Method	Save the method
Curve Report	Produce the graphical curve fit report

Update Calibration Level dialog



Qualifier ratio values are unchanged

Zero Calibration Level dialog



Zero calibration sets all target response values to zero for the selected levels. This will ensure that during update, only response values from the new data are set in the method. If a compound is not found, the response will stay zero.

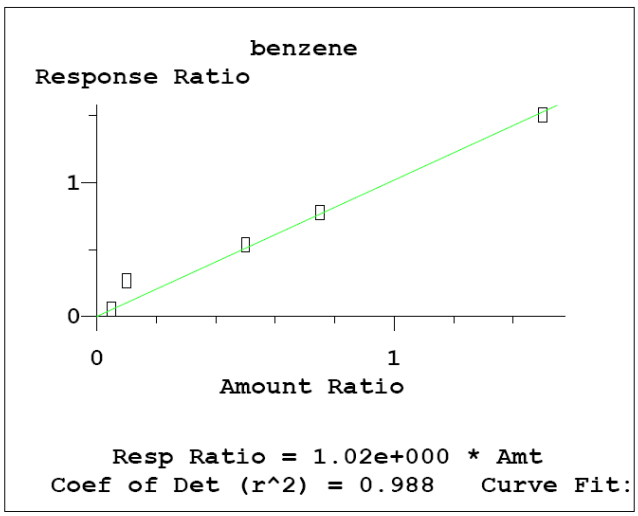
Method Calibration Table Report 1

Method: GAS04.M
CalUpdate: Mon Apr 17 15:37:26 2006
Inst: 5972 - In
Date: Mon Apr 17 16:48:14 2006

LvID	Datafile
A1	STD_A1.D
A2	STD_A2.D
A3	STD_A3.D
A4	STD_A4.D
A5	0002.D
B1	STD_B1.D
B2	STD_B2.D
B3	STD_B3.D
B4	STD_B4.D
B5	STD_B5.D

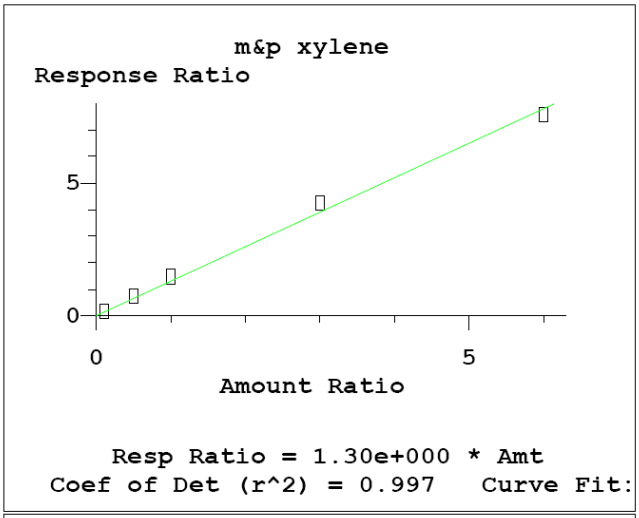
LvID	Amount	Response	N	benzene-d6
A1	2000.0	2839917	1	ISTD has no curve.
A2	2000.0	2800383	1	
A3	2000.0	2696312	1	
A4	2000.0	2666580	1	
A5	2000.0	2657674	1	

LvID	Amount	Response	N
A1	3000.0	4258969	1
A2	1500.0	2176907	1
A3	1000.0	1441676	1
A4	200.0	711291	1
A5	100.0	141234	1

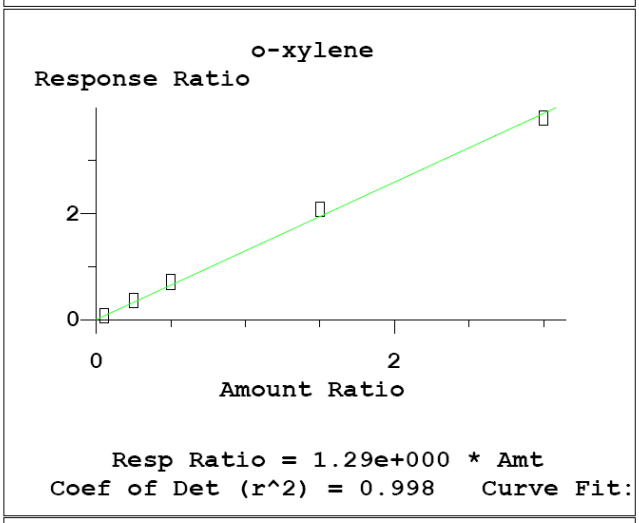


Method Calibration Table Report 2

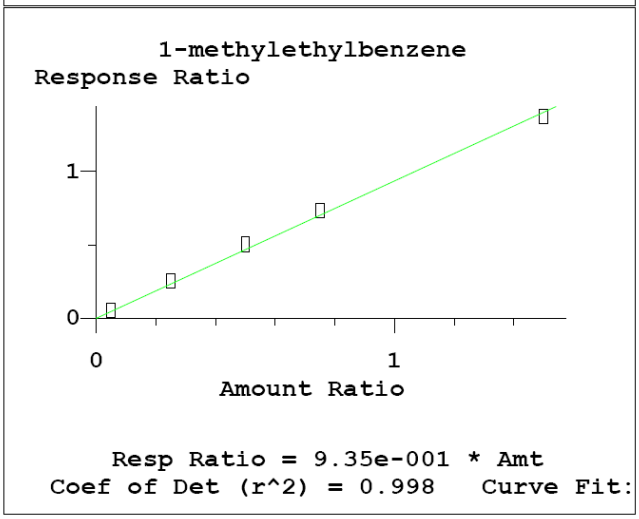
LvID	Amount	Response	N
A1	12000.0	6744337	1
A2	6000.0	3702302	1
A3	2000.0	1301284	1
A4	1000.0	650319	1
A5	200.0	130439	1



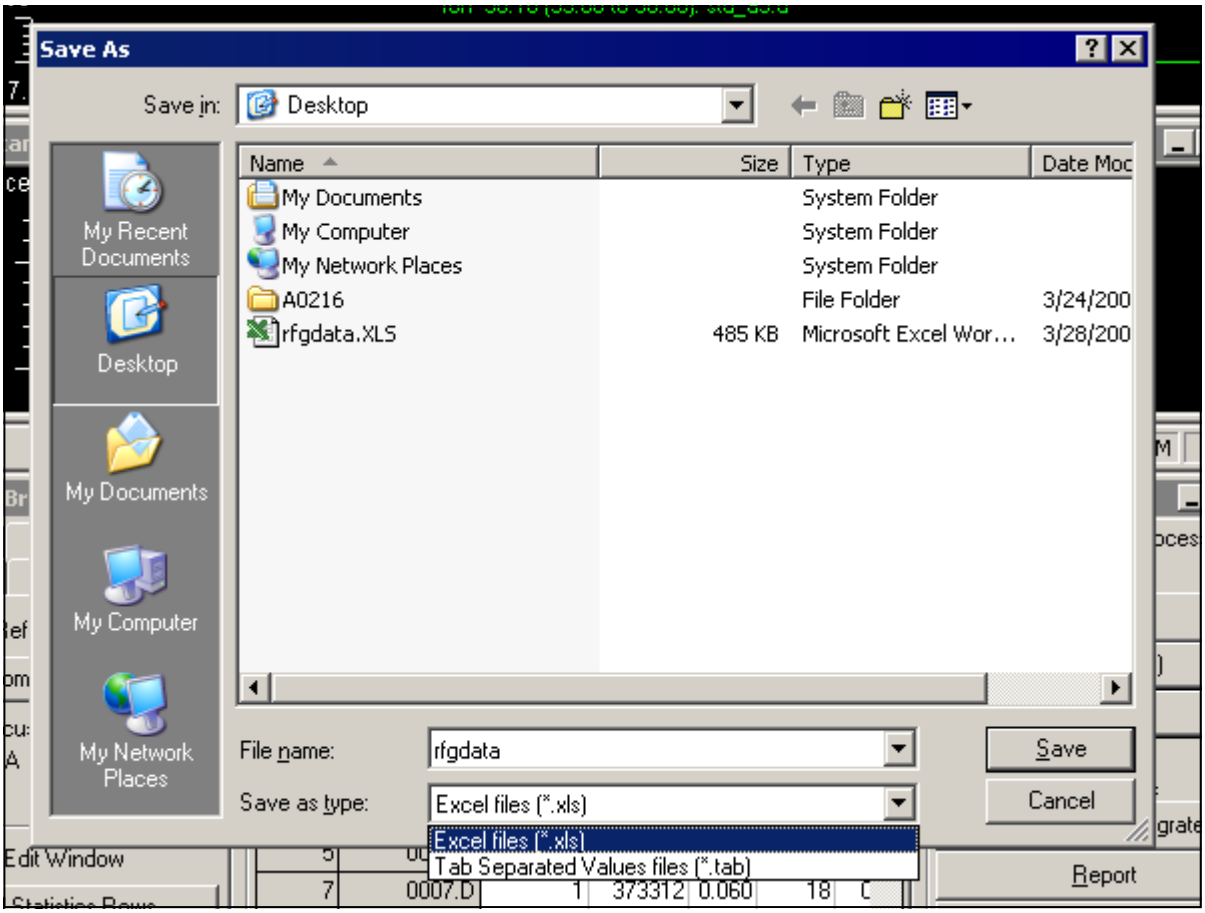
LvID	Amount	Response	N
A1	6000.0	3374554	1
A2	3000.0	1816025	1
A3	1000.0	628074	1
A4	500.0	315853	1
A5	100.0	62825	1



LvID	Amount	Response	N
B1	1500.0	1218600	1
B2	750.0	644864	1
B3	500.0	437043	1
B4	250.0	228307	1
B5	50.0	44889	1



Exporting



The default export format is the one that is selected under Options. With the 'Save as type' selection the default can be overruled.

Platform for LIMS submission

Quant Browser can be extended to submit the results in to a LIMS system. That will reduce operator handling and ensure data traceability and data integrity.
A LIMS Export Module can be custom made that:

1. Submits the results directly to a database by an SQL statement
2. Posts data in to web-based LIMS connector
3. Writes the data in a file and eventually executes a LIMS client program.

Data for LIMS can be encrypted or appended by a CRC string to ensure data integrity.

Please ask your vendor for a quote.