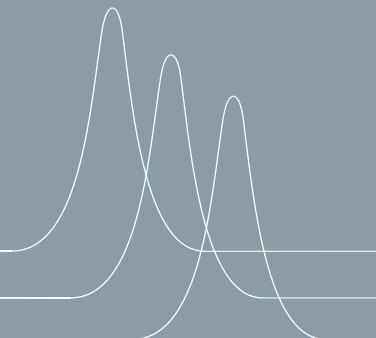




CSQUANT

Data mining software for
LC-MS/MS analysis



Take control of your data!

Fast & easy data evaluation
for Chromsystems assays

Simplifies and accelerates

- Drugs of Abuse Testing
- Amino Acid Analysis (AAA)
- Therapeutic Drug Monitoring

Stop searching – start finding!

Clinical laboratories performing routine LC-MS/MS are required to evaluate large amounts of data – and the more analytes an assay covers, the more data there is to consider.

One example is the Chromsystems **MassTox**[®] Drugs of Abuse Testing assay that covers more than 100 analytes. A batch of 25 samples produces **more than 10,000 data points to consider**: analyte concentration confirmation by ion ratio, internal standard peak areas, quality control values as well as the identification of peaks that require more attention.

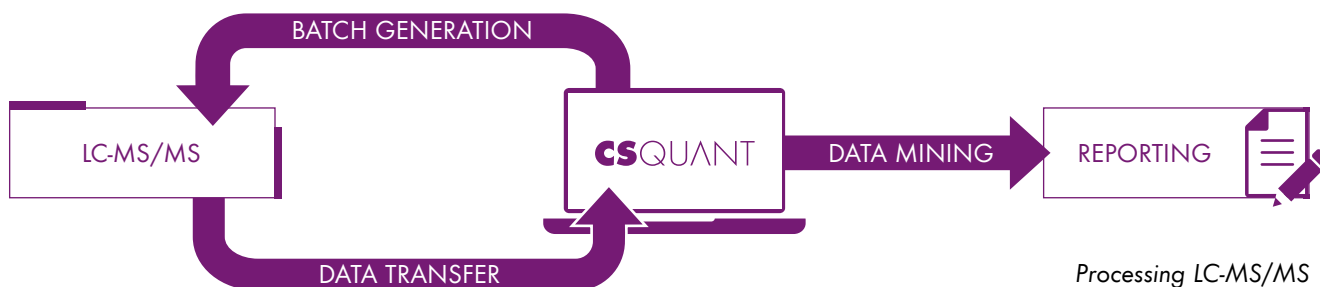
CSQUANT is here to help: it simplifies and accelerates the evaluation of the data generated by Chromsystems assays – from batch generation through data mining to reporting.

Users of **CSQUANT** immediately realised a reduction of the time for data analysis by up to 50%.

Get in touch
for a software
demonstration with
your local sales
representative.



Customers confirm: **CSQUANT** can double the speed of complex LC-MS/MS data analysis.



Processing LC-MS/MS data with **CSQUANT**.

CSQUANT simplifies your LC-MS/MS data analysis

Looking for a run that needs more attention? You would like to see how the internal standard performs over time? How did all the quality control samples perform? The same questions every day, but still a time-consuming and laborious process that feels almost like finding a needle in a haystack!

Not anymore. **CSQUANT** summarises all data for you and supports the user by flagging those that need further attention. Additionally, all analyte groups can be filtered exactly as you require. In other words, **CSQUANT** saves you time, while also minimising the risk of errors.

CSQUANT flags controls and samples automatically upon certain criteria. Find more on page 4.

An overview of the **CSQUANT** workflow

Batch Builder

Generation of batch files with automated spreading of calibrators and controls

Quality Control Index

At a glance visualisation of how the quality control measurements performed

Quality Control Summary

Overview of performance data of measured calibrator and control samples

Samples Tab

Overview of the patient sample results with flagging for better orientation

Sample Summary

Overview of analytes in each sample

Reporting

Automated reports for each sample

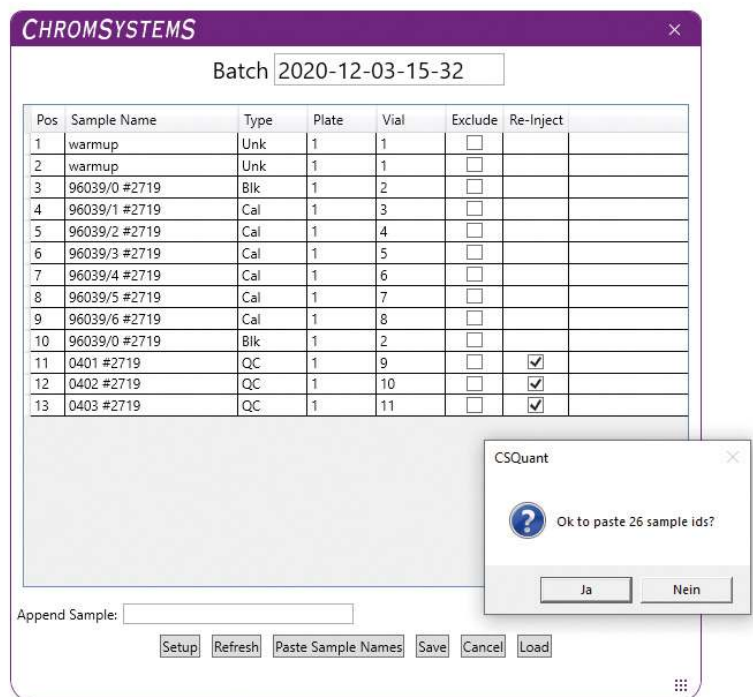
More details can be found on the following pages

The Batch Builder





When using the Batch Builder component for the first time, laboratories define the frequency of quality controls and calibrators. The Batch Builder spreads them accordingly in the batch file.

Easy 3-step action:

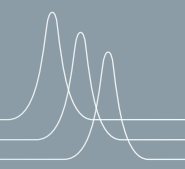
1. Define frequency of calibrators and quality controls.
(direct data import of target values)
2. Copy your sample IDs from a Microsoft Excel sheet or a LIMS system. The IDs can be directly imported via barcode scanning as well.
3. Paste sample IDs into the batch builder.



CSQUANT flagging legend

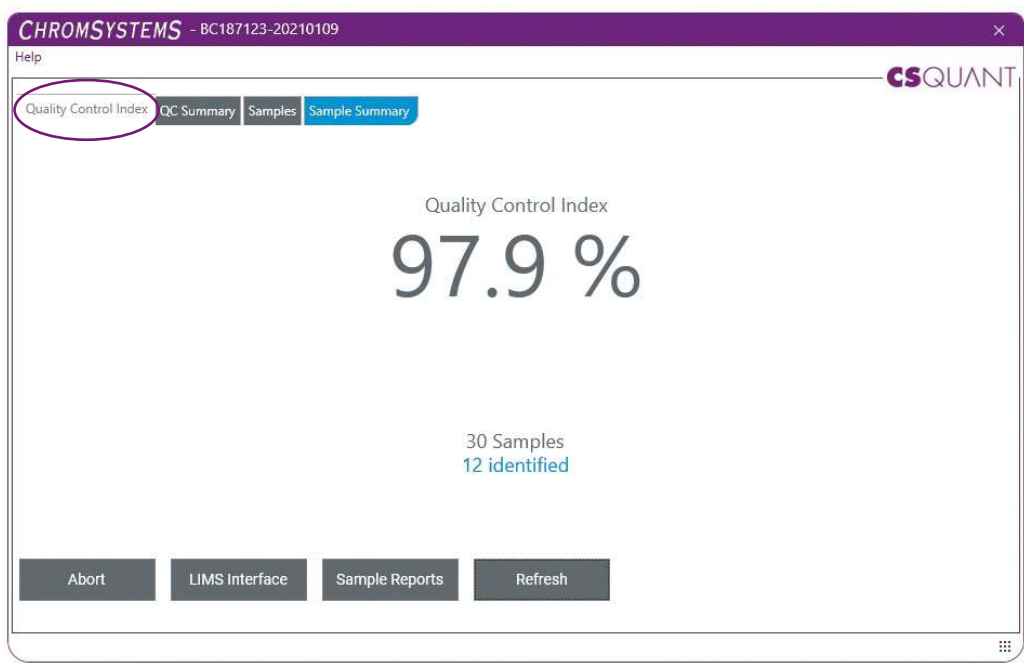
-  Reported concentration is between upper *cut-off* value and *ULOQ*
-  Reported concentration is between *LLOQ* and lower *cut-off* value
-  Reported concentration is higher than *ULOQ*
- <123 Reported concentration is lower than *LLOQ*
-  One or more of the performed checks failed

For a more detailed introduction to the **CSQUANT** flagging, please contact your local sales representative or write to: support@chromsystems.com

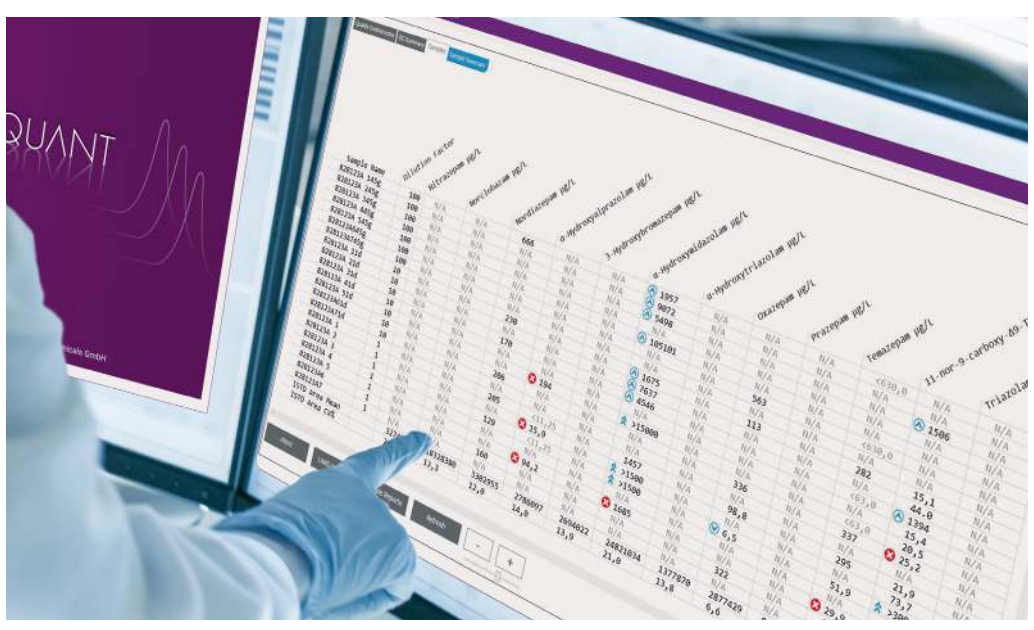


The Quality Control Index

After the LC-MS/MS run, **CSQUANT** provides a Quality Control Index. Based on whether the target values of all quality control samples were reached (accuracy) it allows laboratories to assess the performance of the analysis at a glance.



The Quality Control Index shows at a glance how well the run performed.



The flagging eases identification of conspicuous samples.

The Quality Control Summary

QC and calibrator samples that may need more attention are flagged and can therefore be swiftly identified. With one click, users are also able to identify the potential problem with the sample and can go back to the original mass spectrometry data, for re-integration or further analysis. After correction, the revised mass spectrometry data are automatically updated in **CSQUANT**.

CHROMSYSTEMS - 20200509rs_DoA

Help

Quality Control Index **QC Summary** Samples Sample Summary

Sample Name	Dilution Factor	Measurement	DesmethylFlunitrazepam	Estazolam	Flunitrazepam	Flurazepam	Lorazepam		
96039/1 #2719	1		+2.1 %	+5.4 %	+1.8 %	+2.4 %	-1.1 %		
96039/2 #2719	1		-0.7 %	-2.9 %	+0.2 %	-1.9 %	+1.4 %		
96039/3 #2719	1		-5.8 %	-14.0 %	-9.4 %	-4.6 %	+0.7 %		
96039/4 #2719	1		-4.0 %	-3.9 %	+1.5 %	-3.5 %	+1.2 %		
96039/5 #2719	1		+2.2 %	-0.3 %	+0.6 %	+1.9 %	+0.2 %		
96039/6 #2719	1		+6.2 %	+15.6 %	+5.3 %	+5.7 %	-2.4 %		
0401 #2719	1		-2.6 %	-5.6 %	+0.1 %	-2.8 %	-1.3 %		
0402 #2719	1		-5.1 %	-7.4 %	-4.3 %	-4.5 %	-3.7 %		
0403 #2719	1		+0.8 %	+4.1 %	+0.1 %	-1.7 %	-4.7 %		
Ion Ratio	Mean		0.429	0.811	0.385	0.418	0.932	0.967	0.2
ISTD Area	Mean		7233022	10093527	13632902	73473958	2281067	7124343	831
ISTD Area	CV%		9.2	24.5	22.1	9.6	8.6	11.5	11.1

Details

Sample 96039/6 #2719

Analyte: Estazolam 1

Dilution Factor: 1

Accuracy

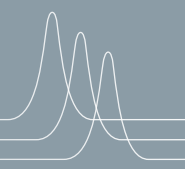
Detailed information on each sample with just one click.

Additionally the performance of the internal standard of quality controls over time can be monitored. This lends full control over the mass spectrometry setup and ensures potential problems are identified quickly.

Samples Evaluation Criteria used by **CSQUANT**

Criteria	Evaluation
Ion Ratio	Quantifier and qualifier ion ratios of samples vs average ion ratio of QCs
Cut-offs	Cut-offs pre-defined for each analyte
Peak Area Internal Standard	Measured IS peak area vs average IS peak area
LLOQ	Calculated concentration vs pre-defined LLOQ
ULOQ	Calculated concentration vs pre-defined ULOQ

CSQUANT gathers the complete mass spectrometry data and evaluates automatically based on these user-defined criteria.



The Samples Tab

Automatic flagging for better navigation.

Patient results are shown in a separate tab. Those that are relevant or need attention are flagged (legend on page 4) accordingly. Filtering by analyte group or respective flagging also simplifies the navigation through the sample data.

CHROMSYSTEMS - 20200509rs_DoA

Help

Quality Control Index QC Summary **Samples** Sample Summary

Sample Name	Dilution Factor	3-Hydroxybromazepam µg/L	α-Hydroxymidazolam µg/L	α-Hydroxytriazolam µg/L	Oxazepam µg/L	Prirazepam µg/L	Temazepam µg/L	11-nor-9-carboxy-Δ ⁹ -THC	Trt
828123A61d	10	N/A	N/A	N/A	336	N/A	337	25.2	
828123A71d	10	N/A	N/A	N/A	N/A	N/A	N/A	N/A	
828123A 1	1	N/A	1457	N/A	98.8	N/A	295	21.9	
828123A 2	1	N/A	>1500	N/A	N/A	N/A	N/A	73.7	
828123A 3	1	N/A	>1500	N/A	6.50	N/A	51.9	>300	
828123A 4	1	N/A	N/A	N/A	N/A	N/A	N/A	16.2	
828123A 5	1	N/A	1685	N/A	N/A	N/A	29.9	23.3	
828123A6	1	N/A	N/A	N/A	322	N/A	310	28.2	
828123A7	1	N/A	N/A	N/A	N/A	N/A	N/A	0.549	
ISTD Area Mean		2694022	24821034	1377870	2877429	8457786	8233621	2742287	

Sort by

- Amphetamines
- Opiates/Opioids
- Benzodiazepines
- Barbiturates
- Cocaine
- Booster
- Others
- Cannabinoids
- Z-Drugs

Errors

OK

Results can easily be filtered, for example by analyte group shown here for the Chromsystems assay **MassTox®** Drugs of Abuse Testing.

The Sample Summary

The Sample Summary tab contains an overview of the number of analytes per group that exceeds the lower cut-off value in each sample, allowing a quick and detailed insight into the patient results. For the **MassTox®** Drugs of Abuse Testing assay, the tab shows positive samples for each analyte group and each patient sample.

CHROMSYSTEMS - 20200509rs_DoA

Help

Quality Control Index QC Summary Samples **Sample Summary**

Sample Name	Dilution Factor	Opiates/Opioids	Benzodiazepines	Cocaine	Booster	Cannabinoids
828123A 445g	100					
828123A 545g	100	2				
828123A645g	100	1			1	
828123A745g	100					
828123A 11d	10	5				1
828123A 21d	10	2				1
828123A 31d	10	1	3	2		1
828123A 41d	10					1
828123A 51d	10		2			1
828123A61d	10		3	1	1	
828123A71d	10					

Sample Summary

Sample 828123A 11d

Component	Result
Midazolam	62.6
Nordiazepam	230
Oxazepam	113
Temazepam	282
α-Hydroxymidazolam	1675

Detailed view of a specific sample.



Last but not least: Reporting

CSQUANT lets you generate a report at any stage of the data mining and evaluation process. It contains information about the result file from the mass spectrometry system and lists all pre-configured analytes and corresponding concentrations. The report can be printed or saved as a PDF.

Your local sales representative will be happy to answer any questions you might have concerning **CSQUANT**.

For further information, please visit:
chromsystems.com/csquant



Ordering Information

Order No.

CSQUANT Base Package (one or more Add-ons required) Includes: installation, training, instruction manual	42999
CSQUANT Add-on for <i>MassTox</i>[®] Drugs of Abuse Testing in Urine	42996
CSQUANT Add-on for <i>MassChrom</i>[®] Amino Acid Analysis in Plasma/Serum	42975
CSQUANT Add-ons for <i>MassTox</i>[®] TDM Series A Parameter Sets:	
Neuroleptics 1/ <i>EXTENDED</i> in Serum/Plasma	42912
Antidepressants 1/ <i>EXTENDED</i> in Serum/Plasma	42913
Neuroleptics 2/ <i>EXTENDED</i> 2 in Serum/Plasma	42914
Antidepressants 2/ <i>Psychostimulants/EXTENDED</i> in Serum/Plasma	42915
Mycophenolic Acid in Serum/Plasma	42916
Benzodiazepines 1 in Serum/Plasma	42917
Benzodiazepines 2 in Serum/Plasma	42918
Tricyclic Antidepressants TCA 1 in Serum/Plasma	42919
Tricyclic Antidepressants TCA 2 in Serum/Plasma	42920
Antiepileptic Drugs/ <i>EXTENDED</i> in Serum/Plasma	42921
Antimycotic Drugs/ <i>EXTENDED</i> in Serum/Plasma	42922
Antiarrhythmic Drugs in Serum/Plasma	42923
Anti-HIV Drugs in Serum/Plasma	42924



CSQUANT online

Full **LIMS** (Laboratory Information Management System) integration upon request!

Please Note: **CSQUANT** is not intended to give the user any information, recommendation or advice on any diagnostic decision on patients. For research use only, not for use in diagnostic procedures.

Compatible LC-MS software: Sciex Analyst[®] (from version 1.6/MD version 1.6), Sciex Multiquant[™] (from version 3.0/MD version 3.0), Waters MassLynx[™] incl. TargetLynx[™] (from version 4.2)

We are continuously working to enhance the compatibility of **CSQUANT**.

If your software is not currently listed, please contact our technical support team.

Our license conditions apply to the acquisition and use of **CSQUANT**. For further information visit www.chromsystems.com/csquant-licence