



MultiQuant™ Software Version 2.0: The Next Generation in Quantitative Data Processing

Mauro Aiello, Ph.D.

Product Manager, Pharmaceutical Quantitation



Overview

- Challenges in data processing
- The MultiQuant™ Software solution
- Powerful features for fast and efficient data processing
- Productivity gains
- Regulatory compliance features

Challenges in Quantitative Data Processing

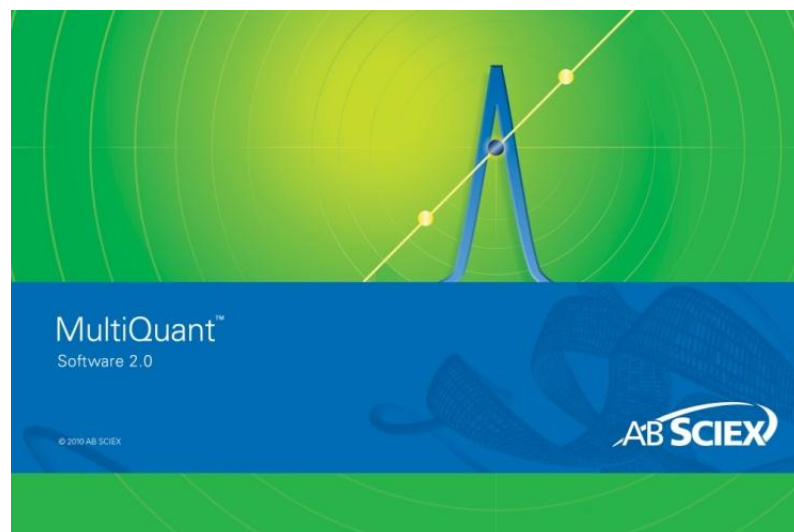
- Recent technology advances have resulted in much higher sample throughput
 - UHPLC
 - Multiplexing / staggered injection techniques
 - Automated sample preparation
- And more analytes per sample
 - Faster scanning instruments (QTRAP[®] 5500 Systems)
 - Automated compound optimization (DiscoveryQuant[™] Software)
 - *Scheduled* MRM[™] Algorithm
- Net result: Much more data is generated

Quantitative Data Processing Remains a Significant Bottleneck

- Time consuming and labor intensive steps of data processing
 - Chromatographic peak integration
 - Peak review
 - Adjust integration parameters when needed, then reintegrate
 - Evaluate standards and QC samples against acceptance criteria
 - Work is multiplied by the number of analytes
- As well as....
 - Determine which samples require re-injection
 - Samples above the upper limit of quantitation need to be diluted
 - Documentation, review and audit trail / e-signatures.
- In spite of improvements in instrumentation and workflows, data processing has remained essentially the same.

MultiQuant™ Software Version 2.0

- Next generation data processing software from AB SCIEX
- Processes multiple data types including MRM, accurate mass Full Scan and MRM³
- Intuitive workspace for data processing
- Very powerful for handling multiple analytes
- Advanced Query and metric plot functionality to speed up data review
- Powerful audit trail and compliance features for GLP laboratories.
- Advanced SignalFinder™ algorithm delivers reliable integration the first time and extends dynamic range



User Friendly Interface

- Powerful yet easy to use
- Faster training of new users
- More efficient data review

Results

Index	Sample Name	Sample Type	IS	Component Name	IS Name	Actual Concentration	Area	Height	IS Area	Retention Time	Used	Calculated Concentration	Accuracy
1	STD 1	Standard	<input type="checkbox"/>	minoxidol	rescinnamine	2.00	4.268e4	5.973e3	6.046e5	1.17	<input checked="" type="checkbox"/>	2.432e0	121.59
5	STD 1	Standard	<input type="checkbox"/>	minoxidol	rescinnamine	2.00	4.091e4	6.317e3	5.952e5	1.05	<input checked="" type="checkbox"/>	2.375e0	118.77
9	STD 2	Standard	<input type="checkbox"/>	minoxidol	rescinnamine	4.00	7.170e4	1.085e4	5.563e5	1.04	<input checked="" type="checkbox"/>	4.196e0	104.89
13	STD 2	Standard	<input type="checkbox"/>	minoxidol	rescinnamine	4.00	7.150e4	1.081e4	6.817e5	1.03	<input checked="" type="checkbox"/>	3.469e0	86.73
17	STD 3	Standard	<input type="checkbox"/>	minoxidol	rescinnamine	8.00	1.526e5	2.257e4	6.741e5	1.03	<input checked="" type="checkbox"/>	7.144e0	89.31
21	STD 3	Standard	<input type="checkbox"/>	minoxidol	rescinnamine	8.00	1.405e5	2.055e4	5.780e5	1.03	<input checked="" type="checkbox"/>	7.654e0	95.67
25	STD 4	Standard	<input checked="" type="checkbox"/>	minoxidol	rescinnamine	16.00	2.891e5	4.095e4	5.750e5	1.03	<input checked="" type="checkbox"/>	1.551e1	96.92
29	STD 4	Standard	<input type="checkbox"/>	minoxidol	rescinnamine	16.00	2.921e5	4.186e4	5.994e5	1.04	<input checked="" type="checkbox"/>	1.504e1	94.01
			<input type="checkbox"/>	minoxidol	rescinnamine	32.00	5.890e5	8.057e4	6.210e5	1.04	<input checked="" type="checkbox"/>	2.899e1	90.60
			<input type="checkbox"/>	minoxidol	rescinnamine	32.00	5.757e5	8.558e4	5.760e5	1.05	<input checked="" type="checkbox"/>	3.054e1	95.45
			<input type="checkbox"/>	minoxidol	rescinnamine	64.00	1.249e6	1.832e5	5.587e5	1.03	<input checked="" type="checkbox"/>	6.795e1	106.18
			<input type="checkbox"/>	minoxidol	rescinnamine	64.00	1.122e6	1.633e5	5.578e5	1.04	<input checked="" type="checkbox"/>	6.115e1	95.55

Peak Review

STD 4 - minoxidol [Standard] 210.2 / 164.2 - Mix_batch_1.wif (sample 7)
Area: 2.891e5, Height: 4.095e4, RT: 1.03 min

STD 4 - minoxidol [Standard] 210.2 / 164.2 - Mix_batch_1.wif (sample 8)
Area: 2.921e5, Height: 4.186e4, RT: 1.04 min

Dynamic Linking of Panes

One Click Metric Plots

Dynamic Linking of Panes

MultiQuant 2.0 - [MQ4] Calibration (Example1.MQ2.qsession)

File Edit Process Audit Trail Window Help

Components & Groups IS

All Components

All Internal Standards
rescinnamine

All Analytes
minoxidol
tolbutamide
reserpine

Index	Sample Name	Sample Type	IS	Component Name	IS Name	Actual Concentration	Area	Height	IS Area	Retention Time	Used	Calculated Concentration	Accuracy
14	STD 2	Standard	<input type="checkbox"/>	tolbutamide	rescinnamine	4.00	6.965e3	1.053e3	6.817e5	1.60	<input checked="" type="checkbox"/>	3.809e0	95.23
15	STD 2	Standard	<input type="checkbox"/>	reserpine	rescinnamine	4.00	8.690e3	1.313e3	6.817e5	2.07	<input checked="" type="checkbox"/>	4.105e0	102.63
18	STD 3	Standard	<input type="checkbox"/>	tolbutamide	rescinnamine	8.00	1.357e4	2.047e3	6.741e5	1.60	<input checked="" type="checkbox"/>	6.912e0	86.40
19	STD 3	Standard	<input type="checkbox"/>	reserpine	rescinnamine	8.00	1.414e4	1.875e3	6.741e5	2.07	<input checked="" type="checkbox"/>	6.680e0	83.50
22	STD 3	Standard	<input type="checkbox"/>	tolbutamide	rescinnamine	8.00	1.266e4	1.930e3	5.780e5	1.60	<input checked="" type="checkbox"/>	7.572e0	94.65
23	STD 3	Standard	<input type="checkbox"/>	reserpine	rescinnamine	8.00	1.391e4	1.860e3	5.780e5	2.07	<input checked="" type="checkbox"/>	7.647e0	95.23
26	STD 4	Standard	<input type="checkbox"/>	tolbutamide	rescinnamine	16.00	2.664e4	4.119e3	5.750e5	1.61	<input checked="" type="checkbox"/>	1.511e1	95.23
27	STD 4	Standard	<input type="checkbox"/>	reserpine	rescinnamine	16.00	2.736e4	3.847e3	5.750e5	2.05	<input checked="" type="checkbox"/>	1.501e1	95.23
30	STD 4	Standard	<input type="checkbox"/>	tolbutamide	rescinnamine	16.00	2.841e4	4.256e3	5.994e5	1.63	<input checked="" type="checkbox"/>	1.501e1	95.23
31	STD 4	Standard	<input type="checkbox"/>	reserpine	rescinnamine	16.00	2.898e4	4.132e3	5.994e5	2.09	<input checked="" type="checkbox"/>	1.501e1	95.30
34	STD 5	Standard	<input checked="" type="checkbox"/>	tolbutamide	rescinnamine	32.00	5.609e4	8.421e3	6.210e5	1.61	<input checked="" type="checkbox"/>	3.249e1	90.23
35	STD 5	Standard	<input type="checkbox"/>	reserpine	rescinnamine	32.00	6.622e4	8.885e3	6.210e5	2.07	<input checked="" type="checkbox"/>	3.249e1	104.64

Regression

- Calibration for tolbutamide: $y = 0.00320x + -0.00195$ ($r = 0.99477$) (weighting: $1/x$)
- Calibration for reserpine: $y = 0.00320x + -3.71550e-4$ ($r = 0.99814$) (weighting: $1/x$)

Area Ratio

Concentration Ratio

Apply Manual Integration

Gaussian Smooth Width: 0.0 points

Expected RT: 1.58 min

RT Half Window: 30.0 sec

Update Expected RT: No

Report Largest Peak

Min. Peak Width: 3 points

Min. Peak Height: 0.00

Integration Parameters

Noise Percentage: 40.0 %

Baseline Sub. Window: 2.00 min

Peak Splitting: 2 points

STD 5 - tolbutamide(Standard) 271.3 / 91.1 - Mix_batch_1.wif (sample 9)
Area: 5.609e4, Height: 8.421e3, RT: 1.61 min

STD 5 - reserpine (Standard) 609.4 / 195.0 - Mix_batch_1.wif (sample 9)
Area: 6.622e4, Height: 8.885e3, RT: 2.07 min

Intensity

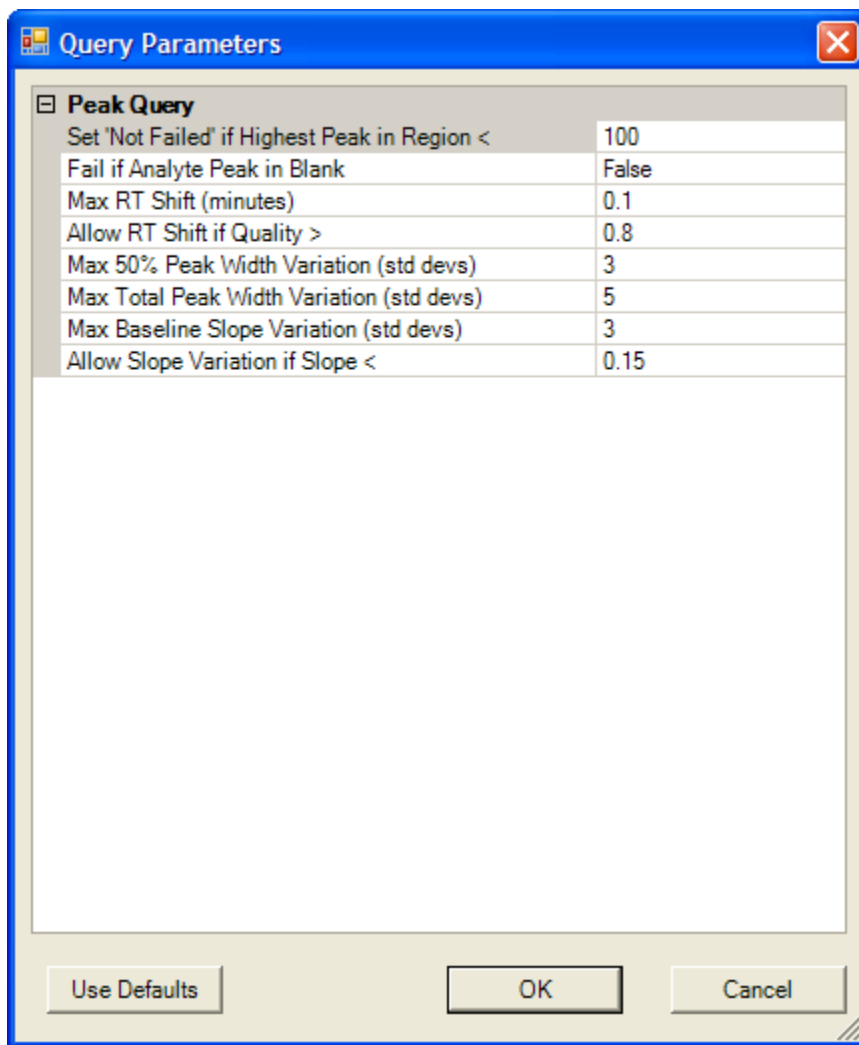
Time, min

Clicking on a point on the calibration curve or metric plot will move results table and peak review to that sample

Queries

- Quickly identify outliers
- Evaluate peak integration
- Evaluate consistency in analyte/IS peak areas when multiple MRMs per analyte is monitored
- Find failed standards or QC samples
- Reduces the need for manual review
- Failed samples are automatically flagged and a reason is provided.

Predefined and Custom Queries



- Many standard queries already included in the software.
- Can contain multiple criteria.
- Tolerances are user defined.
- Custom calculations can be applied.

Peak Query

Automatically Find Poor Integrations or Outliers

MultiQuant 2.0 - [[MQ4] Results Table (training.qsession), Query: Peak Query]

File Edit Process Audit Trail Window Help

Example

Components & Groups IS

All Components

- All Internal Standards
 - Flunitrazepam.IS
 - Nordiazepam.IS
- All Analytes
 - Flunitrazepam
 - Nordiazepam

Index	Sample ID	Sample Type	IS	Component Name	IS Name	Failed Query	Actual Concentration	Area	IS Area	Height	Retention Time	Width at 50%	Used	Calculated Concentration	Accuracy	Peak Failure
1		Double Blank	<input checked="" type="checkbox"/>	Flunitrazepam.IS	N/A	<input type="checkbox"/>	N/A	4.402e1	N/A	4.000e1	0.88	0.02		N/A	N/A	
2		Double Blank	<input checked="" type="checkbox"/>	Nordiazepam.IS	N/A	<input type="checkbox"/>	N/A	2.640e1	N/A	4.000e1	1.18	0.01		N/A	N/A	
3		Double Blank	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	<input type="checkbox"/>	N/A	3.960e1	4.402e1	6.000e1	1.36	0.01	<input checked="" type="checkbox"/>	N/A	N/A	
4		Double Blank	<input type="checkbox"/>	Nordiazepam	Nordiazepam.IS	<input checked="" type="checkbox"/>	N/A	3.964e1	2.640e1	3.637e1	1.70	0.04	<input checked="" type="checkbox"/>	N/A	N/A	RT
5		Double Blank	<input checked="" type="checkbox"/>	Flunitrazepam.IS	N/A	<input type="checkbox"/>	N/A	3.960e1	N/A	4.000e1	1.26	0.03		N/A	N/A	
6		Double Blank	<input checked="" type="checkbox"/>	Nordiazepam.IS	N/A	<input type="checkbox"/>	N/A	2.203e1	N/A	6.000e1	1.13	0.01		N/A	N/A	
7		Double Blank	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	<input type="checkbox"/>	N/A	3.960e1	3.960e1	6.000e1	1.42	0.01	<input checked="" type="checkbox"/>	N/A	N/A	
8		Double Blank	<input type="checkbox"/>	Nordiazepam	Nordiazepam.IS	<input type="checkbox"/>	N/A	3.523e1	2.203e1	6.000e1	1.33	0.01	<input checked="" type="checkbox"/>	N/A	N/A	
9		Blank	<input checked="" type="checkbox"/>	Flunitrazepam.IS	N/A	<input type="checkbox"/>	1.00	1.186e4	N/A	4.533e3	1.05	0.04		N/A	N/A	
10		Blank	<input checked="" type="checkbox"/>	Nordiazepam.IS	N/A	<input checked="" type="checkbox"/>	1.00	1.858e3	N/A	1.040e3	1.39	0.02		N/A	N/A	RT
11		Blank	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	<input checked="" type="checkbox"/>	N/A	7.712e1	1.186e4	1.125e2	1.06	0.02	<input checked="" type="checkbox"/>	< 0	N/A	RT
12		Blank	<input type="checkbox"/>	Nordiazepam	Nordiazepam.IS	<input type="checkbox"/>	N/A	3.960e1	1.858e3	8.000e1	1.41	0.02	<input checked="" type="checkbox"/>	< 0	N/A	
13		Standard	<input checked="" type="checkbox"/>	Flunitrazepam.IS	N/A	<input type="checkbox"/>	1.00	2.546e4	N/A	9.932e3	1.05	0.04		N/A	N/A	
14		Standard	<input checked="" type="checkbox"/>	Nordiazepam.IS	N/A	<input type="checkbox"/>	1.00	4.054e3	N/A	2.260e3	1.40	0.03		N/A	N/A	
15		Standard	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	<input type="checkbox"/>	0.12	9.815e2	2.546e4	4.448e2	1.07	0.04	<input type="checkbox"/>	< 0	N/A	
16		Standard	<input type="checkbox"/>	Nordiazepam	Nordiazepam.IS	<input type="checkbox"/>	0.12	2.201e2	4.054e3	1.600e2	1.42	0.04	<input checked="" type="checkbox"/>	< 0	N/A	
17		Standard	<input checked="" type="checkbox"/>	Flunitrazepam.IS	N/A	<input type="checkbox"/>	1.00	2.623e4	N/A	1.126e4	1.05	0.03		N/A	N/A	
18		Standard	<input checked="" type="checkbox"/>	Nordiazepam.IS	N/A	<input type="checkbox"/>	1.00	4.029e3	N/A	2.160e3	1.40	0.03		N/A	N/A	
19		Standard	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	<input type="checkbox"/>	0.24	1.713e3	2.623e4	7.600e2	1.07	0.03	<input type="checkbox"/>	< 0	N/A	
20		Standard	<input type="checkbox"/>	Nordiazepam	Nordiazepam.IS	<input type="checkbox"/>	0.24	4.072e2	4.029e3	2.340e2	1.41	0.03	<input checked="" type="checkbox"/>	< 0	N/A	
21		Standard	<input checked="" type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	<input type="checkbox"/>	1.00	2.597e4	N/A	9.674e3	1.05	0.04		N/A	N/A	
22		Standard	<input checked="" type="checkbox"/>	Nordiazepam	Nordiazepam.IS	<input type="checkbox"/>	1.00	4.195e3	N/A	2.420e3	1.40	0.03		N/A	N/A	
23		Standard	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	<input type="checkbox"/>	0.49	3.335e3	2.597e4	1.608e3	1.07	0.04	<input type="checkbox"/>	4.258e-2	8.69	
24		Standard	<input type="checkbox"/>	Nordiazepam	Nordiazepam.IS	<input type="checkbox"/>	0.49	5.636e2	4.195e3	3.400e2	1.41	0.03	<input checked="" type="checkbox"/>	7.880e-2	16.08	
25		Standard	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	<input type="checkbox"/>	1.00	2.509e4	N/A	9.820e3	1.05	0.04		N/A	N/A	
26		Standard	<input type="checkbox"/>	Nordiazepam	Nordiazepam.IS	<input type="checkbox"/>	1.00	4.094e3	N/A	2.430e3	1.40	0.03		N/A	N/A	
27		Standard	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	<input type="checkbox"/>	0.98	5.851e3	2.509e4	2.500e3	1.07	0.04	<input checked="" type="checkbox"/>	4.640e-1	47.34	
28		Standard	<input type="checkbox"/>	Nordiazepam	Nordiazepam.IS	<input type="checkbox"/>	0.98	1.114e3	4.094e3	5.600e2	1.41	0.03	<input checked="" type="checkbox"/>	5.303e-1	54.11	
29		Standard	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	<input type="checkbox"/>	1.00	2.545e4	N/A	9.931e3	1.05	0.04		N/A	N/A	
30		Standard	<input checked="" type="checkbox"/>	Nordiazepam.IS	N/A	<input type="checkbox"/>	1.00	4.030e3	N/A	2.312e3	1.40	0.03		N/A	N/A	
31		Standard	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	<input type="checkbox"/>	1.95	1.328e4	2.545e4	5.240e3	1.07	0.04	<input checked="" type="checkbox"/>	1.624e0	83.28	
32		Standard	<input type="checkbox"/>	Nordiazepam	Nordiazepam.IS	<input type="checkbox"/>	1.95	2.535e3	4.030e3	1.611e3	1.41	0.02	<input checked="" type="checkbox"/>	1.702e0	87.27	
33		Standard	<input checked="" type="checkbox"/>	Flunitrazepam.IS	N/A	<input type="checkbox"/>	1.00	2.525e4	N/A	9.493e3	1.05	0.04		N/A	N/A	
34		Standard	<input checked="" type="checkbox"/>	Nordiazepam	Nordiazepam.IS	<input type="checkbox"/>	1.00	4.363e3	N/A	2.200e3	1.39	0.03		N/A	N/A	

Failed sample automatically identified and reason provided

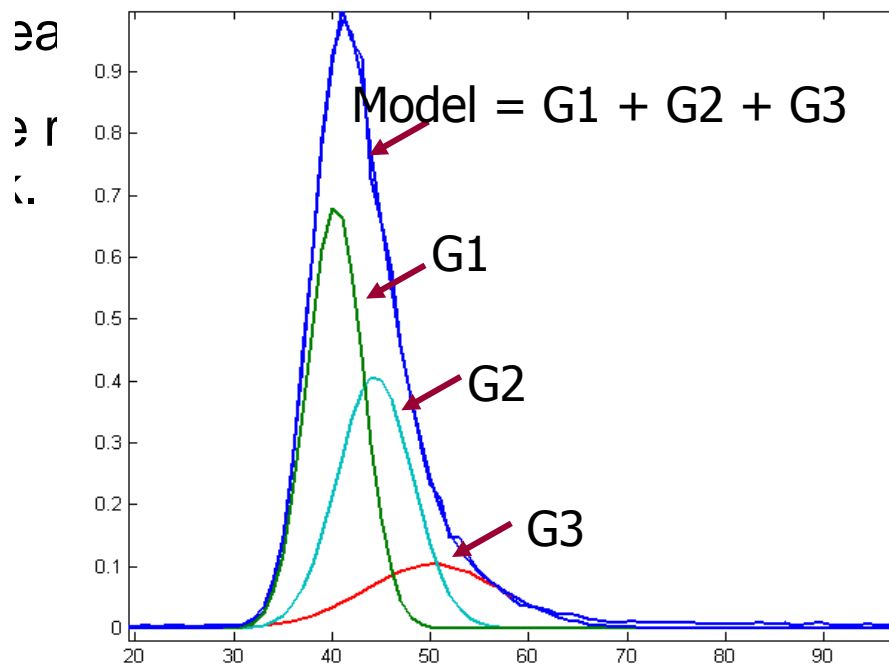
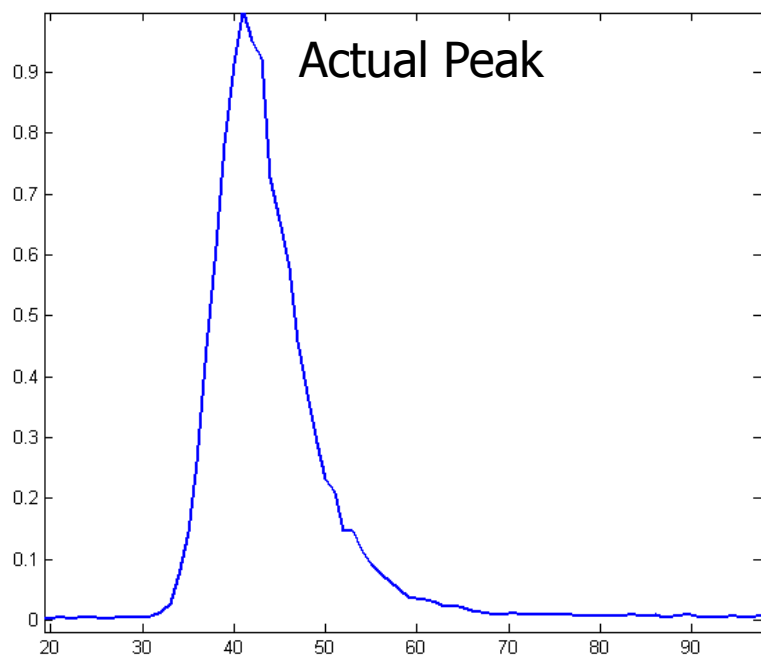
© 2016 AB SCIEX

The SignalFinder™ Integration Algorithm

- A true innovation in peak integration
- Based on the peak modeling approach
- More consistent integration with fewer operator adjusted parameters.
- Peak modeling enables new functionality:
 - Saturation correction
 - Peak deconvolution

How Does Peak Modeling Work ?

- Model is constructed based on a representative peak from the actual raw data.



Advantages of Peak Modeling

SignalFinder™ Integration Algorithm

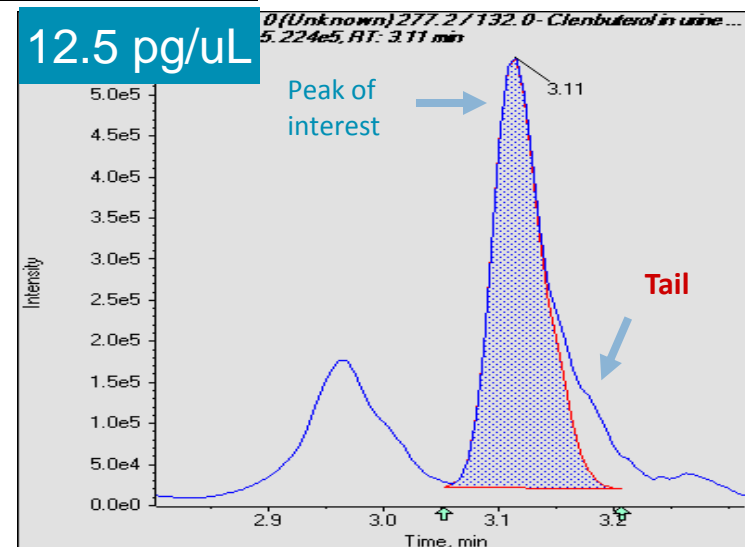
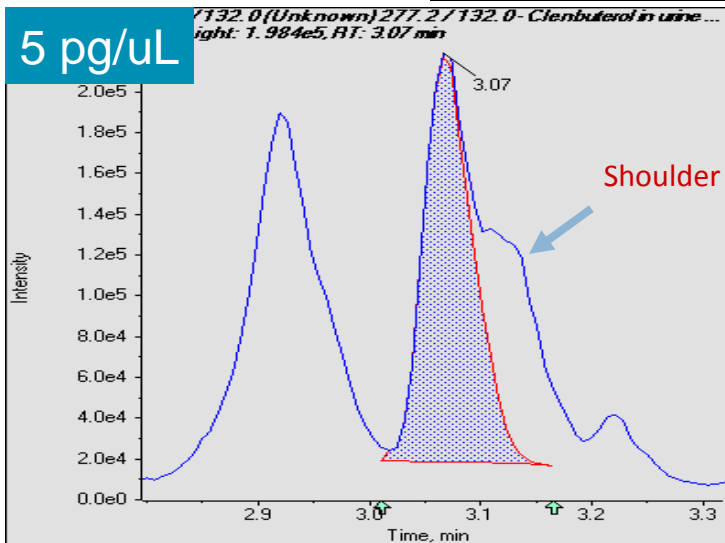
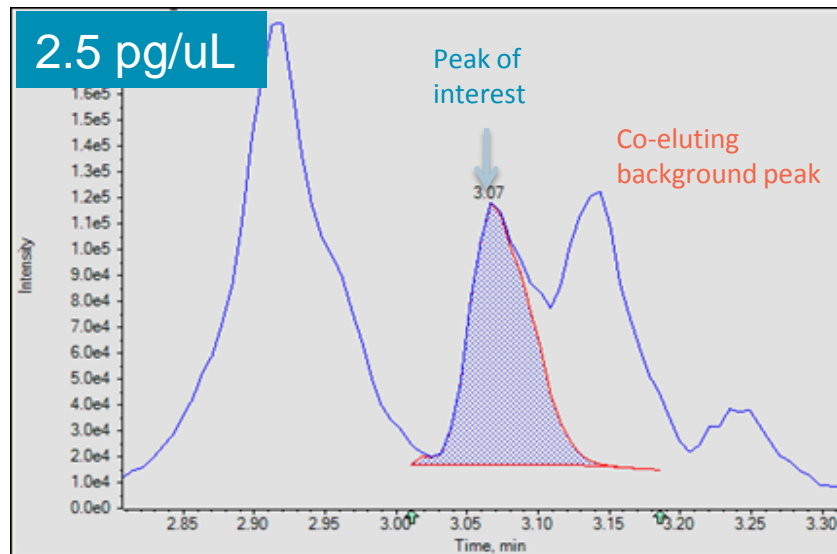
- Robust characterization of the peak shape
- Much better detection of where the peak starts and ends
- Better integration of poorly resolved peaks
- Consistent integration across the concentration range
- Easier to use with fewer parameters
- Less operator intervention to tweak parameters
- Smoothing is not required

Evaluation of Integration Consistency

		IntelliQuan			SignalFinder		
		Response	Each QC	Data Set	Response	Each QC	Data Set
		cps	%CV (n=20)	%CV (n=20)	cps	%CV (n=20)	%CV (n=20)
MRM #1	QC1	9.99E+05	3.3	3.2	9.97E+05	3.3	3.3
	QC2	7.58E+05	2.5	35.2	9.88E+05	2.5	2.5
	QC3	4.36E+04	2.2	33.9	5.71E+04	2.2	2.2
	QC4	9.38E+03	2.5	23.4	1.15E+04	2.4	2.4
	QC5	3.25E+03	3.8	52.0	3.61E+03	3.3	3.3
MRM #2	QC1	9.98E+05	2.9	6.7	1.01E+06	2.8	2.8
	QC2	8.79E+05	2.8	19.2	1.00E+06	2.7	2.7
	QC3	2.44E+03	3.0	19.9	5.78E+04	2.7	2.7
	QC4	5.05E+04	4.7	20.0	1.09E+04	4.4	4.4
	QC5	9.23E+03	8.3	17.8	3.24E+03	7.0	7.0

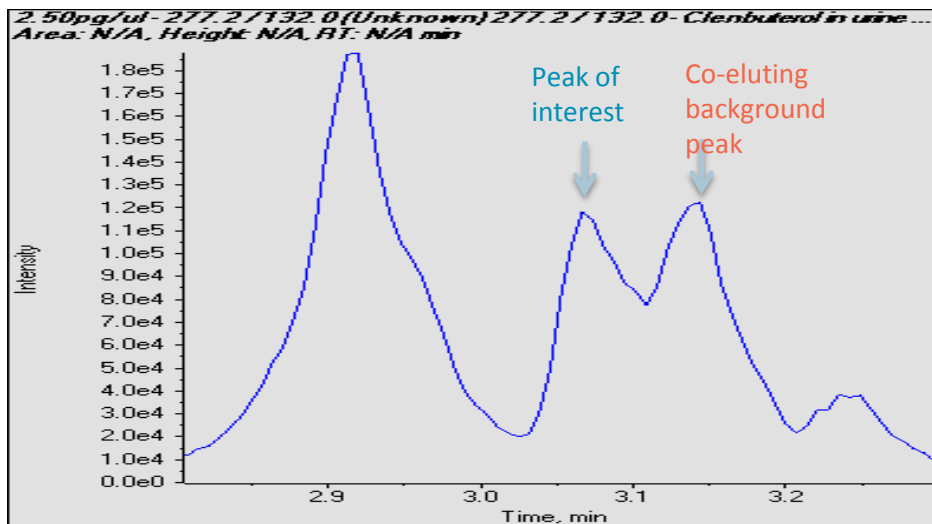
- SignalFinder™ integration algorithm performed significantly better across the concentration range without adjusting the integration parameters.

More Consistent Integration Across a Wide Range

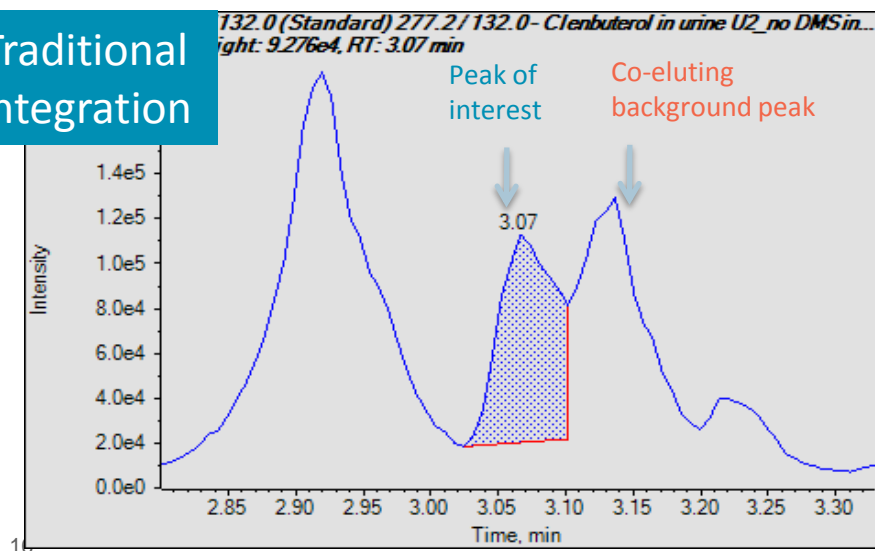


Peak Deconvolution Capability

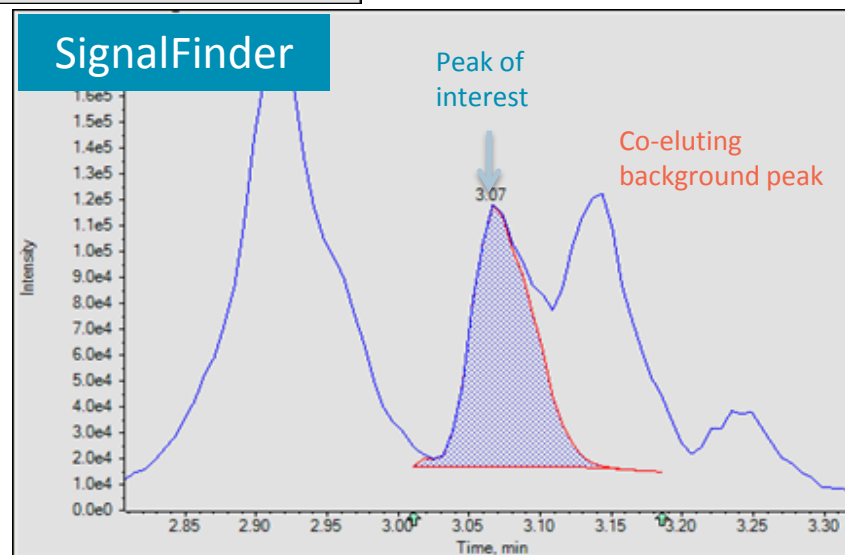
Highly Selective Integration of Poorly Resolved Peaks



Traditional Integration



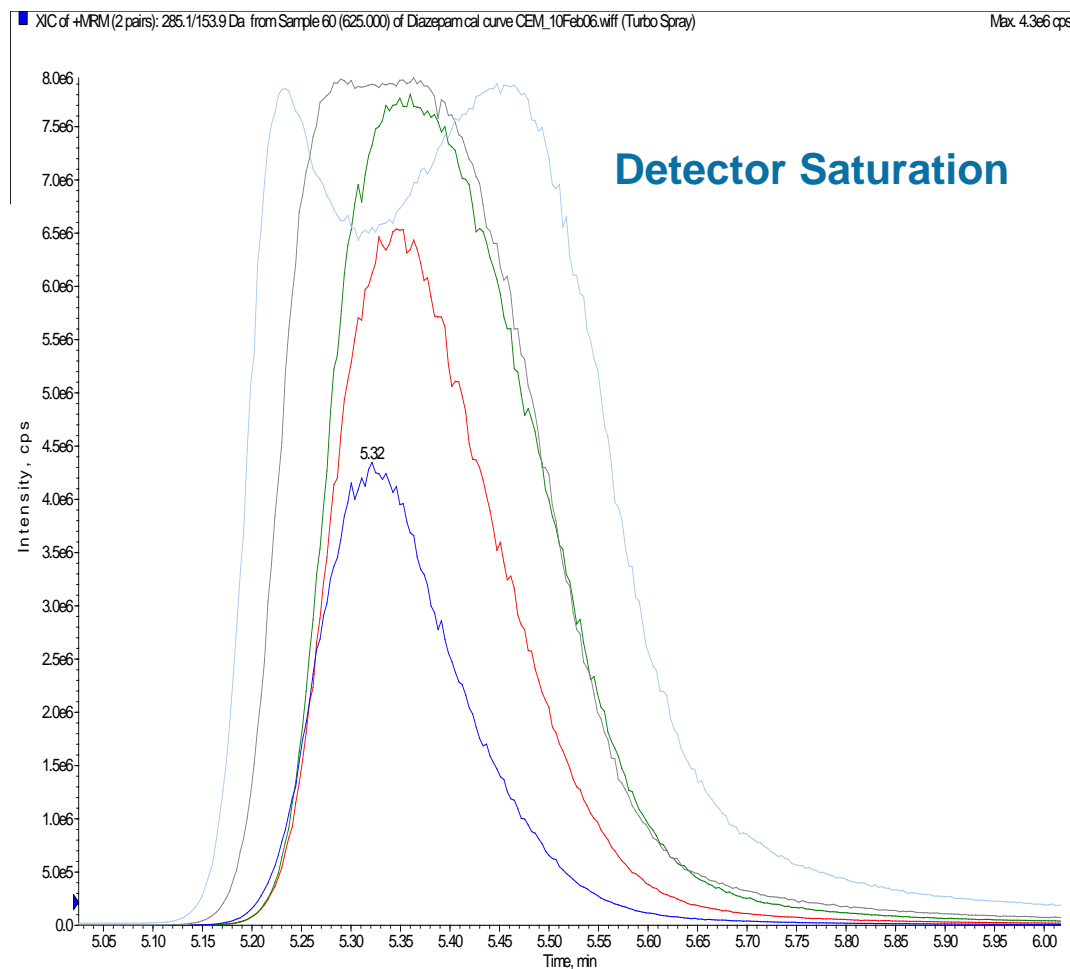
SignalFinder



Saturation Correction

- Use of peak modeling in SignalFinder™ integration algorithm allows unique new capabilities such as optional saturation correction.
- Capability to correct for the saturation of detector response
- Can significantly increase linear dynamic range when deviation is caused by detector saturation.

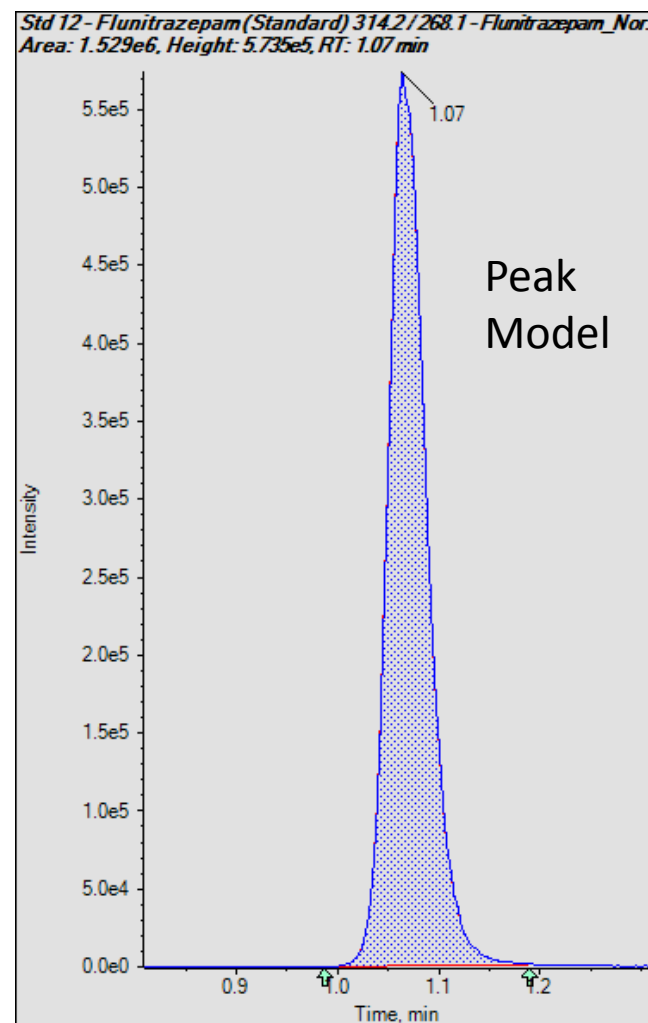
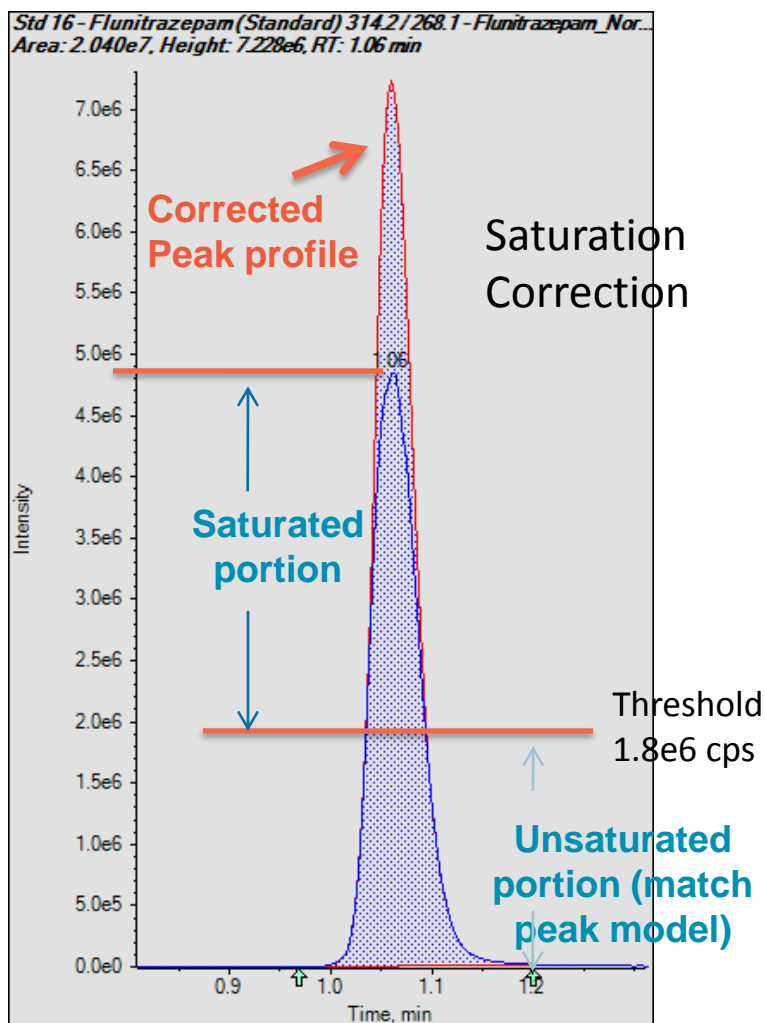
Detector Saturation



- Response flattens as concentration increases
- Peak width also increases
- Peak modeling can account for both phenomena

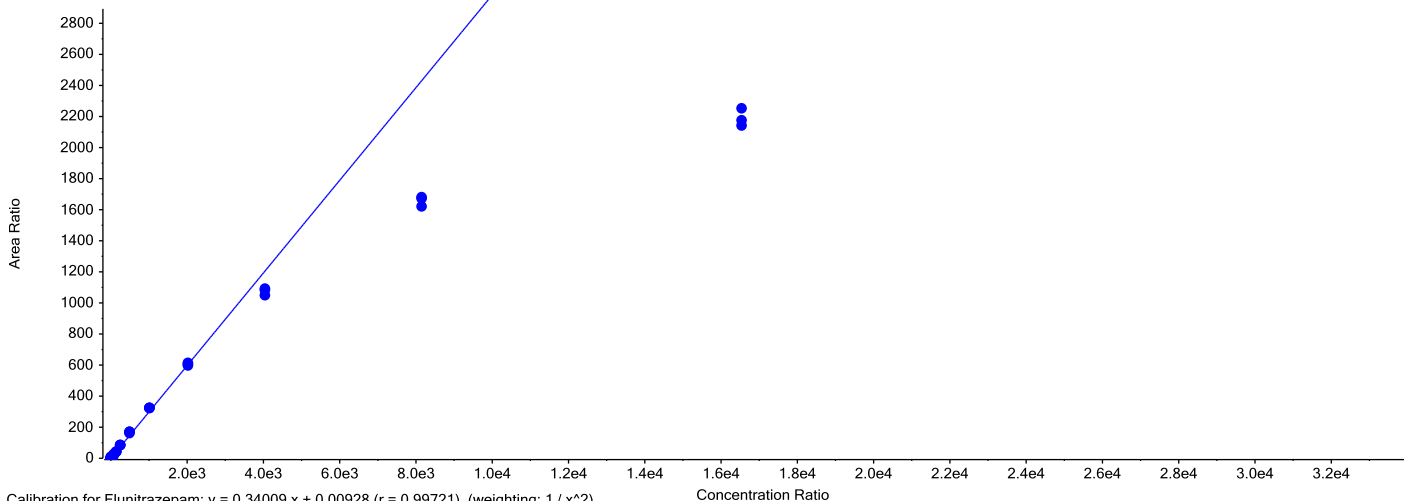
Detector Saturation Correction

Using SignalFinder™ Integration Algorithm

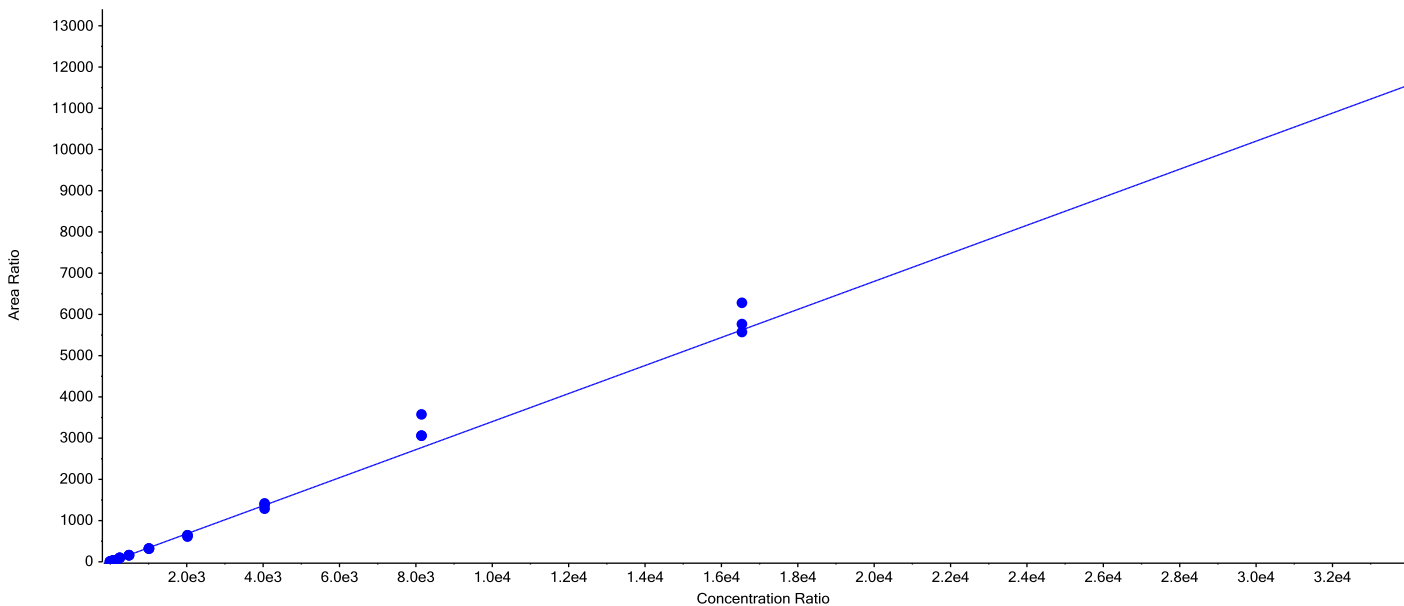


Flunitrazepam with and without correction

Calibration for Flunitrazepam: $y = 0.29825x + 0.01123$ ($r = 0.96106$) (weighting: $1/x^2$)



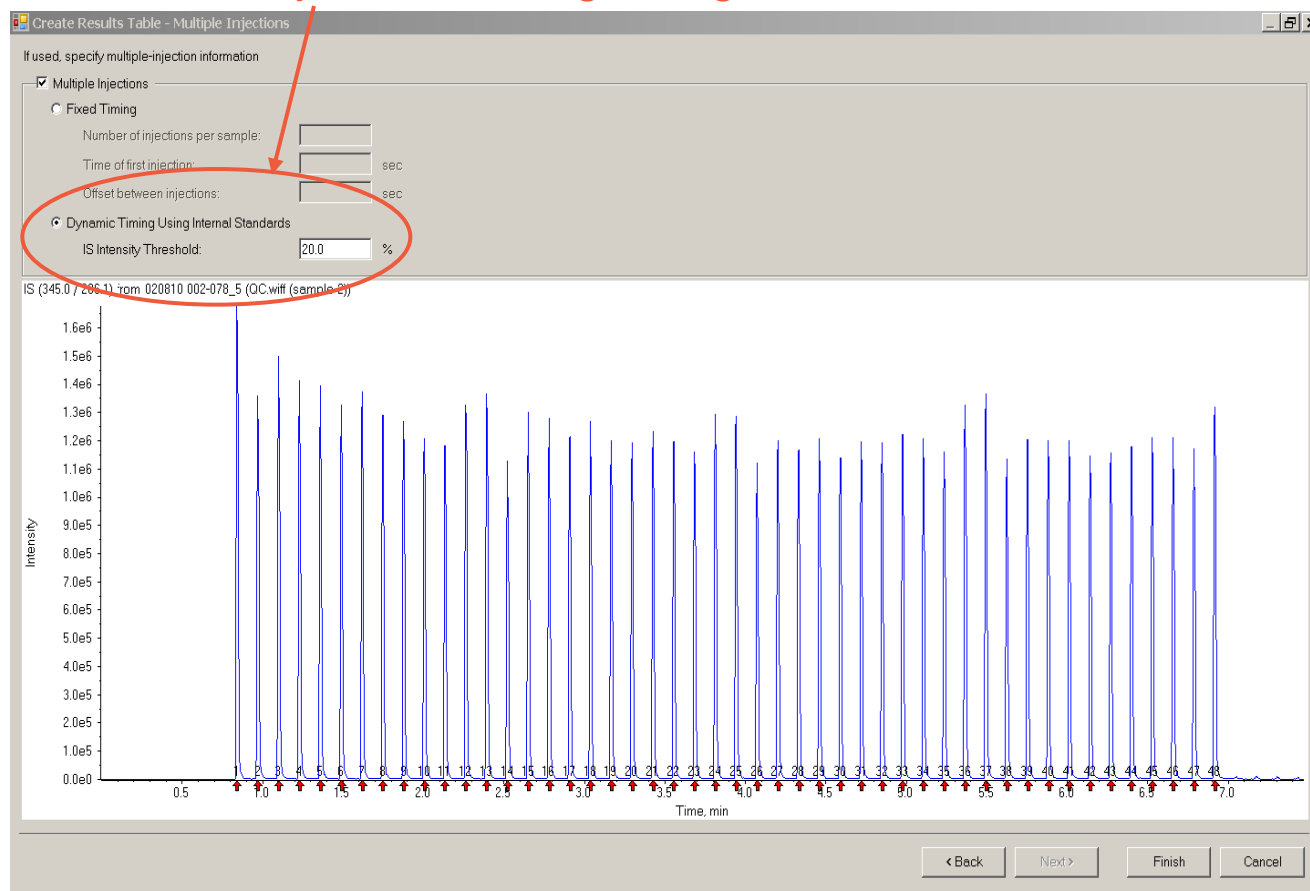
Calibration for Flunitrazepam: $y = 0.34009x + 0.00928$ ($r = 0.99721$) (weighting: $1/x^2$)



Multiple Injections Per Data File

- Rapid injection systems for very high throughput assays
- Multiple injections in the same data file
- Examples: ADME assays such as CYP inhibition and metabolic stability

Dynamic Timing Using IS



Versatile Functions

- External Calibration
 - Can quantify one MRM transition against another
 - Radiolabelled compound quantified against non-labeled standard curve
 - Quantify an endogenous species against a standard curve generated using a stable isotope labeled internal standard.
- Custom Report Generation
 - Pre-configured templates provided for most common report formats
 - Templates can be easily modified or created from scratch
 - Report output in PDF format

Summary of Productivity Gains

- Shorter training time for new users due to ease of use
- Greater consistency in data analysis
- Reduced need for adjustment of integration parameters
- Fast and objective data review using queries and metric plots
- Reduced need for dilutions and re-injections with saturation correction.
- Significant time savings reported for real world high throughput ADME assays¹.

(1) S. Crathern et al, "Automation of Integrated LC-MS/MS Peak Quality Assurance and Analytical Run Quality Control," ASMS 2009.

Compliance Features

- New audit trail with robust management and precise control
- All versions of the results are stored
 - Hyperlinked to the audit trail
 - Quickly see the data before and after a change
- Audit trail search capability
 - Search for specific events across all results tables in a project
 - Track a sample across multiple results tables to identify re-injections.
- Results table locking and secure LIMS export
- Faster training of new operators and more consistency

Audit Trail Viewer

- Shows events and the associated data
- Displays the data before and after the audited change
- Results table and peak review automatically linked to the audit trail.

Audit Trail Viewer

Audit Trail Results Project: Example Session: Example1 MQ2

Find: Go Next Prev Filter... Remove Filter Print... Export...

View updated on: 01/19/2010 18:37:59 (GMT-05:00)

Save Event	Description	Session	Reason	Full User Name	E-Signature
01/19/2010 18:37:54	The session file 'C:\Analyst Data\Projects\Example\Results\Example1 MQ2.qsession' has been modified.	Example1 MQ2		Not Available	No
01/19/2010 18:37:30	Manually integrated - QC 2 of minoxidol		Manual integration	Not Available	Yes
01/19/2010 18:29:23	The session file 'C:\Analyst Data\Projects\Example\Results\Example1 MQ2.qsession' has been saved.	Example1 MQ2		Not Available	No

Results Table Comparison Column Settings... Synchronized

Example1 MQ2: Results Table of the selected Save Event [01/19/2010 18:37:54]

Inde	Sample Name	Sample Type	IS	Component Name	IS Name	Actual Concentra	Area	Height	IS Area	Retentio Time	Used
79	QC 2	Quality Contr	<input type="checkbox"/>	reserpine	rescinnamine	24.00	4.258e4	5.698e3	6.456e5	2.04	<input checked="" type="checkbox"/>
80	QC 2	Quality Contr	<input checked="" type="checkbox"/>	rescinnamine	N/A	1.00	6.456e5	7.234e4	N/A	2.27	<input type="checkbox"/>
81	QC 2	Quality Contr	<input checked="" type="checkbox"/>	minoxidol	rescinnamine	24.00	1.703e5	3.964e4	5.833e5	1.03	<input checked="" type="checkbox"/>

Example1 MQ2: Previous version of the Results Table of the selected Save Event [01/19/2010 18:29:23]

Inde	Sample Name	Sample Type	IS	Component Name	IS Name	Actual Concentra	Area	Height	IS Area	Retentio Time	Used
79	QC 2	Quality Contr	<input type="checkbox"/>	reserpine	rescinnamine	24.00	4.258e4	5.698e3	6.456e5	2.04	<input checked="" type="checkbox"/>
80	QC 2	Quality Contr	<input checked="" type="checkbox"/>	rescinnamine	N/A	1.00	6.456e5	7.234e4	N/A	2.27	<input type="checkbox"/>
81	QC 2	Quality Contr	<input checked="" type="checkbox"/>	minoxidol	rescinnamine	24.00	4.165e5	6.097e4	5.833e5	1.04	<input checked="" type="checkbox"/>

Peak Cal. Curve

QC 2 - minoxidol (Quality Control) 210.2 / 164.2 - Mi...
Area: 1.703e5, Height 3.964e4, RT: 1.03 min

QC 2 - minoxidol (Quality Control) 210.2 / 164.2 - Mi...
Area: 4.165e5, Height 6.097e4, RT: 1.04 min

SW: 0.0
RT: 1.01
RTW: 15.0
LRT: No
RLP: Yes
MPW: 3
MPH: 200.00
Ns%: 40.0
BSW: 2.00
PSF: 2

Advanced Audit Trail Search Capability

- Track a single sample across multiple batches
- Search for a specific audit event such as manual integrations or method changes across multiple result tables.
- Audit trail will show results before and after the change
- Feature results in significantly faster QA review

Filter Audit Trail Events [Clear]

Find instances where:
 Session is contains <all sessions>

And where:
 Sample Name is contains Sample 1

And where:
 Reason is contains Re-injection

And where:
 <No filter> is contains

And where time and date are:
 From: Tuesday, February 23, 2010 12:00:00 AM
 To: Tuesday, February 23, 2010 11:59:59 PM

[OK] [Cancel]

Advanced Audit Trail Search Capability

Audit Trail Viewer

Project: Demo Session: <Filter defined>

Find: Go Next Prev

View updated on: 01/20/2010 10:43:25 (GMT-05:00) Filter: Session is <all sessions> AND Description contains **Manually integrated** Save events returned: 4

Save Event	Description	Session	Reason	Full User Name	E-Signature
01/20/2010 10:42:54	The session file 'D:\Analyst Data\Projects\Demo\Results\RT1.qsession' has been modified.	RT1		pqs1 user	No
Change Event					
Change Event Details					
01/20/2010 10:42:54	Manually integrated - <i>Sample 2 of rescinnamine</i>		Reason	Full User Name	E-Signature
Change Event Details					
01/20/2010 10:42:52	The scan changed from 207 (intensity of 0) to scan 246 (intensity of 3485.636). Area changed from "566358.309" to "507629.046" counts (10% decrease).				
01/20/2010 10:42:48	Manually integrated - <i>STD 4 of rescinnamine</i>			pqs1 user	No
Change Event Details					
01/20/2010 10:42:47	The scan changed from 201 (intensity of 571.879) to scan 237 (intensity of 3621.899). Area changed from "575022.635" to "511342.488" counts (11% decrease).				
01/20/2010 10:42:44	Manually integrated - <i>QC 1 of rescinnamine</i>			pqs1 user	No
Change Event Details					
01/20/2010 10:42:43	The scan changed from 203 (intensity of 365.98) to scan 238 (intensity of 3110.828). Area changed from "573330.917" to "511405.304" counts (11% decrease).				
01/20/2010 10:42:25	The session file 'D:\Analyst Data\Projects\Demo\Results\RT2.qsession' has been modified.	RT2		pqs1 user	No
Change Event					
Change Event Details					
01/20/2010 10:42:25	Manually integrated - <i>QC 3 of tolbutamide</i>			pqs1 user	No
Change Event Details					
01/20/2010 10:42:23	The scan changed from 146 (intensity of 80.04) to scan 171 (intensity of 1440.727). Area changed from "164527.234" to "147993.912" counts (10% decrease).				
01/20/2010 10:42:02	The session file 'D:\Analyst Data\Projects\Demo\Results\RT3.qsession' has been modified.	RT3		pqs1 user	No
Change Event					
Change Event Details					
01/20/2010 10:42:02	Manually integrated - <i>STD 6 of minoxidol</i>			pqs1 user	No
Change Event Details					
01/20/2010 10:42:01	The scan changed from 91 (intensity of 555.071) to scan 117 (intensity of 8326.06). Area changed from "1249280.479" to "1134360.775" counts (9% decrease).				
01/20/2010 10:41:47	The session file 'D:\Analyst Data\Projects\Demo\Results\RT4.qsession' has been modified.	RT4		pqs1 user	No
Change Event					
Change Event Details					
01/20/2010 10:41:47	Manually integrated - <i>STD 7 of reserpine</i>			pqs1 user	No

Results Table Comparison Column Settings... Synchronized

RT1: Results Table of the selected Save Event [01/20/2010 10:42:54]

Index	Sample Name	Sample ID	Sample Type	IS	Component Nam	IS Name	Component Group Name	Actual Concentratio	Area	Height	Retention Time	W at
145	Sample 2		Unknown	<input type="checkbox"/>	minoxidol	rescinnamine		N/A	4.888e5	7.090e4	1.04	0.10
146	Sample 2		Unknown	<input type="checkbox"/>	tolbutamide	rescinnamine		N/A	4.317e4	6.961e3	1.63	0.09
147	Sample 2		Unknown	<input type="checkbox"/>	reserpine	rescinnamine		N/A	4.395e4	6.205e3	2.12	0.10
148	Sample 2		Unknown	<input checked="" type="checkbox"/>	rescinnamine	N/A		1.00	5.076e5	5.880e4	2.34	0.13
149	Sample 3		Unknown	<input type="checkbox"/>	minoxidol	rescinnamine		N/A	7.023e5	9.815e4	1.04	0.10

RT1: Previous version of the Results Table of the selected Save Event [01/20/2010 10:40:01]

Index	Sample Name	Sample ID	Sample Type	IS	Component Nam	IS Name	Component Group Name	Actual Concentratio	Area	Height	Retention Time	W at
145	Sample 2		Unknown	<input type="checkbox"/>	minoxidol	rescinnamine		N/A	4.888e5	7.090e4	1.04	0.10
146	Sample 2		Unknown	<input type="checkbox"/>	tolbutamide	rescinnamine		N/A	4.317e4	6.961e3	1.63	0.09
147	Sample 2		Unknown	<input type="checkbox"/>	reserpine	rescinnamine		N/A	4.395e4	6.205e3	2.12	0.10
148	Sample 2		Unknown	<input checked="" type="checkbox"/>	rescinnamine	N/A		1.00	5.664e5	6.044e4	2.34	0.13
149	Sample 3		Unknown	<input type="checkbox"/>	minoxidol	rescinnamine		N/A	7.023e5	9.815e4	1.04	0.10

Peak **Cal. Curve**

Sample 2 - rescinnamine (Unknown) 635.4 / 221.2 - Mix_batch_1.wiff (sample...
Area: 5.076e5, Height: 5.880e4, RT: 2.34 min

SW: 0.0
RT: 2.30
RTW: 30.0
URT: No
RLP: Yes
MPW: 3
MPH: 0.00
NS: 40.0
BSW: 2.00
PSF: 2

Sample 2 - rescinnamine (Unknown) 635.4 / 221.2 - Mix_batch_1.wiff (sample...
Area: 5.664e5, Height: 6.044e4, RT: 2.34 min

SW: 0.0
RT: 2.30
RTW: 30.0
URT: No
RLP: Yes
MPW: 3
MPH: 0.00
NS: 40.0
BSW: 2.00
PSF: 2

Grouped Audit Events

- Allows the capture of multiple auditable events with a single e-signature.
- Speeds up data processing and allows for more audited events without sacrificing usability.
- Individual date and time stamp for every event
- Option to cancel and discard changes

E-Signature Required

Integration parameters changed for sample - *STD 7 of minoxidol*

Date and Time	Description
01/25/2010 14:33:51	Min. Peak Height changed from 0 to 200. Area changed from "2381225.169" to "2381225.169" counts (0% decrease).
01/25/2010 14:33:42	RT Half Window changed from 30 to 15 sec. Area changed from "2381225.169" to "2381225.169" counts (0% decrease).
01/25/2010 14:33:36	Expected RT changed from 1.03 to 1.01 min. Area changed from "2381225.169" to "2381225.169" counts (0% decrease).

E-Signature:

Reason: Date and Time: 01/25/2010 14:46 (GMT-05:00)

Password: Full User Name: John Doe

User Name: DOMAIN/johndoe

Results Locking

- Prevents unauthorized changes to the results
- Locking can be required prior to exporting or printing
- Security permission required to unlock

MultiQuant 2.0 - [[M04] Results Table (training.qsession - locked)]

File Edit Process Audit Trail Window Help

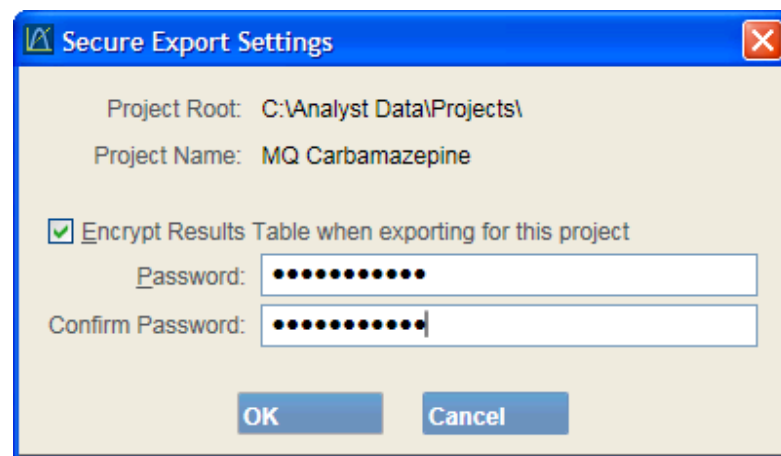
Components & Groups IS #

Index	Sample Name	Sample ID	Sample Type	IS	Component Name	IS Name	Actual Concentration	Area	IS Area	
3	Double Blank		Double Blank	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	N/A	3.960e1	4.402e1	6.000e1	6.000e1	6.000e1								
7	Double Blank		Double Blank	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	N/A	3.960e1	3.960e1	6.000e1	6.000e1	6.000e1								
11	Blank		Blank	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	N/A	7.712e1	1.186e4	1.125e2	1.06									
15	Std 1		Standard	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	0.12	9.815e2	2.546e4	4.448e2										
19	Std 2		Standard	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	0.24	1.713e3	2.623e4	7.600e2										
23	Std 3		Standard	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	0.49	3.335e3	2.597e4				0.04							
27	Std 4		Standard	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	0.98	5.851e3	2.509e4				0.04							
31	Std 5		Standard	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	1.95	1.328e4	2.509e4	3.240e3			0.04							
35	Std 6		Standard	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	3.91	2.586e4	2.256e4	1.014e4			0.04							
39	Std 7		Standard	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	7.81	5.011e4	2.508e4	1.912e4			0.04							
43	Std 8		Standard	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	15.63	1.010e5	2.507e4	3.851e4			0.04							
47	Std 9		Standard	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	31.25	1.967e5	2.536e4	7.594e4			0.04							
51	Std 10		Standard	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	62.50	4.004e5	2.511e4	1.485e5			0.04							
55	Std 11		Standard	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	125.00	7.845e5	2.595e4	2.951e5			0.04							
59	Double Blank		Double Blank	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	N/A	9.555e2	8.361e1	1.212e3	0.60	0.01								
63	Double Blank		Double Blank	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	N/A	7.614e2	4.842e1	1.020e3	1.48	0.00								
67	QC M		Unknown	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	N/A	3.434e5	2.591e4	1.319e5	1.07	0.04								
71	QC H		Unknown	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	N/A	3.363e6	2.518e4	1.296e6	1.07	0.04								
75	QC L		Unknown	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	N/A	3.470e4	2.632e4	1.421e4	1.07	0.04								
79	QC LLOQ		Unknown	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	N/A	1.219e3	2.697e4	5.600e2	1.06	0.04								
83	QC M		Unknown	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	N/A	3.412e5	2.628e4	1.303e5	1.07	0.04								
87	QC H		Unknown	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	N/A	3.428e6	2.625e4	1.290e6	1.07	0.04								
91	QC L		Unknown	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	N/A	3.492e4	2.695e4	1.401e4	1.07	0.04								
95	QC LLOQ		Unknown	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	N/A	1.492e3	2.652e4	6.193e2	1.06	0.07								
99	QC M		Unknown	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	N/A	3.399e5	2.597e4	1.312e5	1.07	0.04								
103	QC H		Unknown	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	N/A	3.429e6	2.591e4	1.295e6	1.07	0.04								
107	QC L		Unknown	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	N/A	3.536e4	2.624e4	1.359e4	1.06	0.04								
111	QC LLOQ		Unknown	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	N/A	1.008e3	2.609e4	6.200e2	1.07	0.03								
115	QC M		Unknown	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	N/A	3.439e5	2.582e4	1.320e5	1.07	0.04								
119	QC H		Unknown	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	N/A	3.386e6	2.560e4	1.317e6	1.06	0.04								
123	QC L		Unknown	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	N/A	3.527e4	2.586e4	1.316e4	1.07	0.04								
127	QC LLOQ		Unknown	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	N/A	1.074e3	2.654e4	5.000e2	1.07	0.04								
131	QC M		Unknown	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	N/A	3.433e5	2.573e4	1.328e5	1.07	0.04								
135	QC H		Unknown	<input type="checkbox"/>	Flunitrazepam	Flunitrazepam.IS	N/A	3.423e6	2.472e4	1.340e6	1.07	0.04								

Results table background turns grey and "locked" is added to header

Additional Compliance Features

- Review Function
 - Adds a specific audit trail event with e-signature to indicate when a session was reviewed and approved.
- Modification Warning
 - Warns users on saving if any samples have modified parameters
 - Prevents accidental modification of samples
- Secure Export
 - Exported text file can be encrypted to prevent tampering with the results after they are exported.



Conclusions

- MultiQuant™ Software 2.0 has the potential to significantly reduce the amount of time required for data processing, review and compliance.
- The software is intuitive and easy-to-use which reduces the amount of time required to train new operators.
- The SignalFinder™ integration algorithm is capable of accurate and consistent integration with fewer parameters and less operator intervention.
- Powerful audit trail and security features ensure data integrity, consistency and regulatory compliance.

Acknowledgments

- Gordana Ivosev
- Lyle Burton
- Richard King and Sue Crathern
- Hesham Ghobarah

Trademarks / Licencing

- For Research Use Only. Not for use in diagnostic procedures.
- The trademarks mentioned herein are the property of AB Sciex Pte. Ltd. or their respective owners. AB SCIEX™ is being used under license.
- © 2010 AB SCIEX.



Thank You