Better Data Faster:
MassHunter Quantitative Analysis

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MassHunter Product Manager

July 29, 2015

Agenda

Brief Introduction

How to fully leverage the information in the raw data during data analysis

Tips and Tricks for fast data review of even thousands of complex samples

Ways to automate peak detection to eliminate the need for manual integration

New features to quickly and automatically create pdf reports

Integrating MassHunter Quantitative Analysis with other laboratory systems

Labs Have More Samples than Ever

Sample Preparation

Chromatographic Separation

Data Analysis

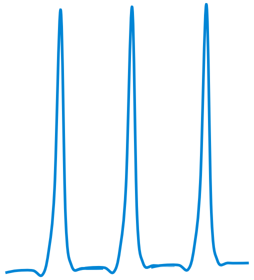
Data Interpretation

Reporting

Agilent MassHunter Suite

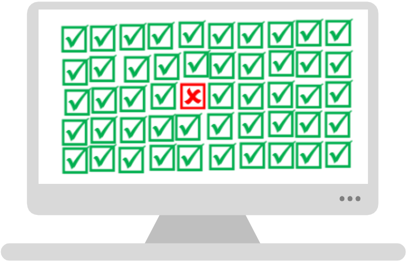
Acquisition

- Agilent LCs, GCs, ICP and MS
- dMRM, tMRM, All Ions, Ion Mobility



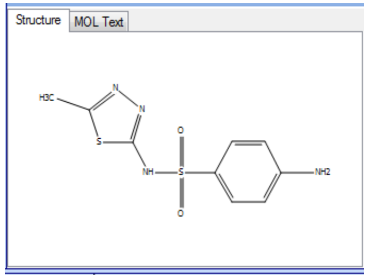
Quantitative Analysis

- High-throughput quantitation
- Easily visualize results (Review-by-Exception)
- Integration with LIMS/LIS
- Custom reports



Qualitative Analysis

- ID and characterize compounds in all markets
- Novel algorithms for feature finding



MassHunter for all your needs

FOOD

ENERGY

PHARMACEUTICAL

ENVIRONMENT

RESEARCH

DIAGNOSTICS

MassHunter Software
One software for all Agilent Mass Spectrometers

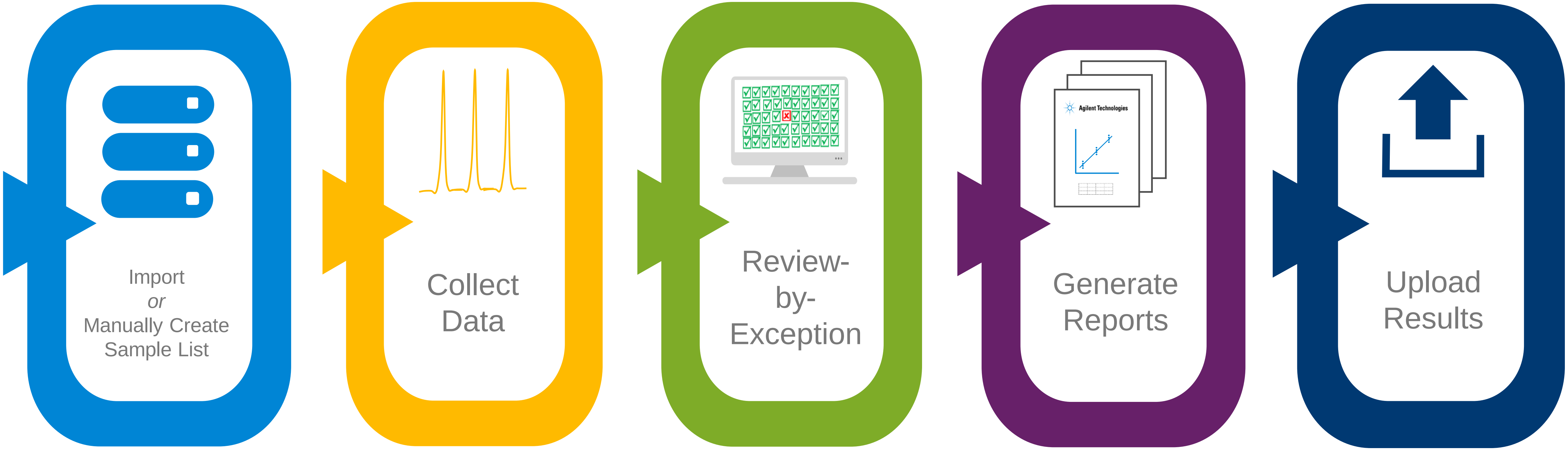
Minimize the training costs and delays – A Single User Experience for all techniques

LC/MS

GC/MS

ICP-MS

MassHunter Quantative Analysis Workflow



Import
or
Manually Create
Sample List

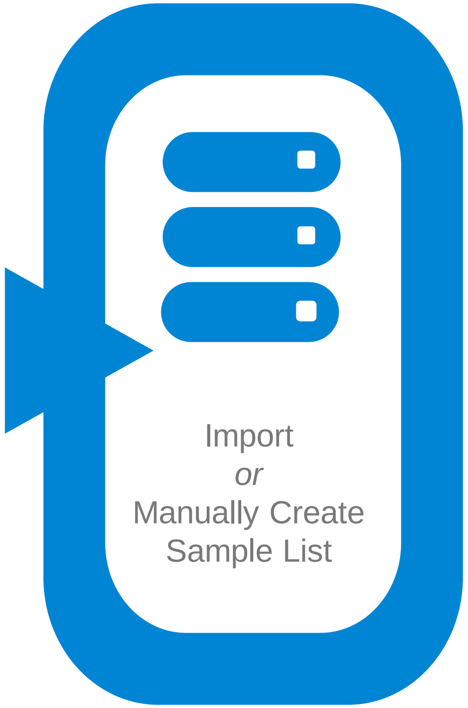
Collect
Data

Review-
by-
Exception

Generate
Reports

Upload
Results

MassHunter Quantative Analysis Workflow

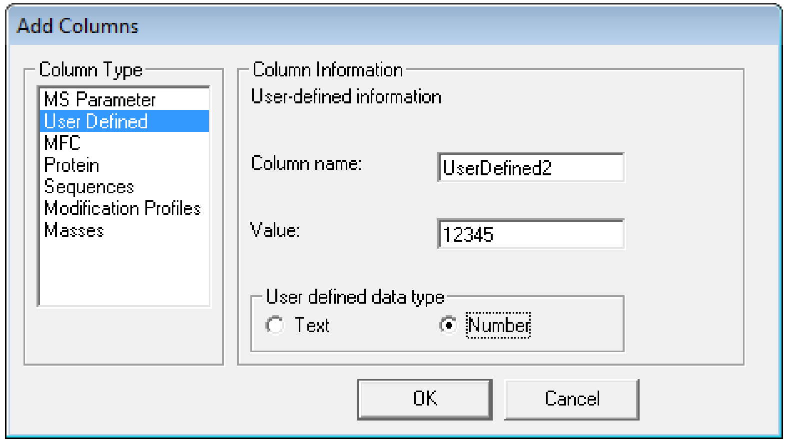


Import
or
Manually Create
Sample List

Including Additional Sample Information about Samples

We have an electronic sample list with sample information (pH, company identifiers, etc.) and we wish this information to appear in the final reports. How can we do this?

- Worklist/Sequence has two columns, “Comments” and “Info.” that will get read by MassHunter Quantitative Analysis.
- 10 additional columns can be created that are labeled “UserDefined, UserDefined1, UserDefined2, etc.”
- Custom columns of other names will get stored in the .D folder but not read by MassHunter Quantitative Analysis to be included in the results for reporting.



Column Type: User Defined

User-defined information

Column name: UserDefined2

Value: 12345

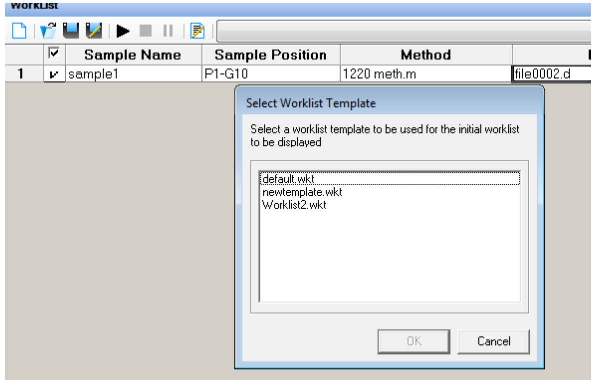
User defined data type: ○ Text ● Number

Remembering Worklist/Sequence Column Layout

We hide, add, or reorder columns but next time MassHunter Acquisition brings it up the original way. How do we get MassHunter to remember these changes?

For LC/MS

- After getting Worklist the way we want, save the Worklist to the MassHunter/Worklist Templates folder
- Rename the file from myworklist.wkl to myworklist.wkt
- To use this template, select New Worklist
- If we don't need more than one, we name it default.wkt



	☑	Sample Name	Sample Position	Method	
1	✓	sample1	P1-G10	1220 meth.m	file0002.d

Select Worklist Template

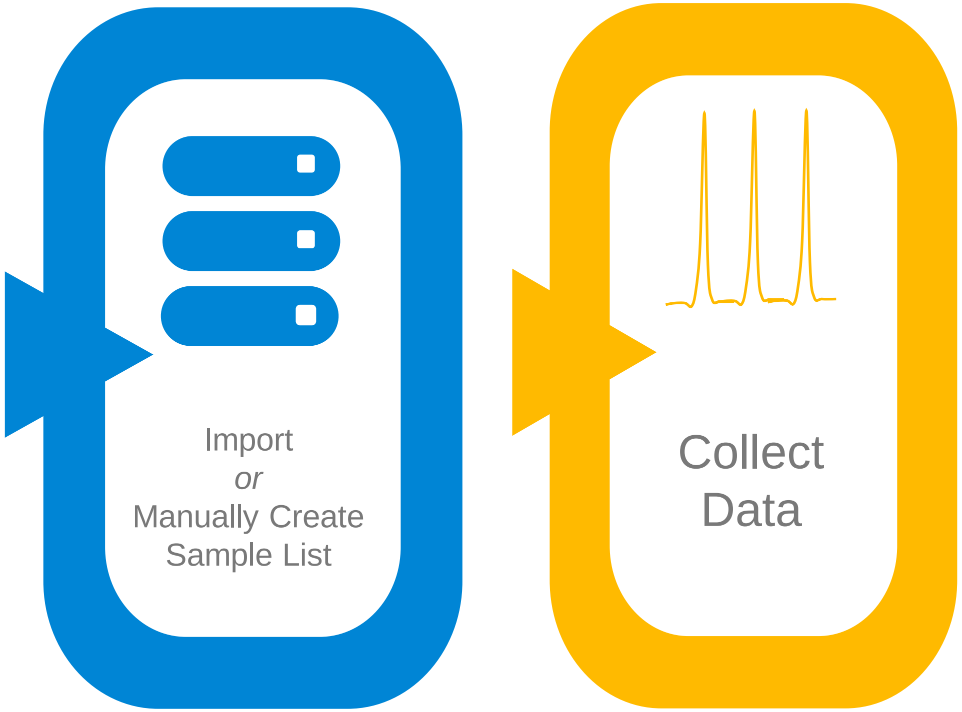
Select a worklist template to be used for the initial worklist to be displayed

default.wkt
newtemplate.wkt
Worklist2.wkt

For GC/MS

- Use the Sequence Table Tools

MassHunter Quantative Analysis Workflow



Import
or
Manually Create
Sample List

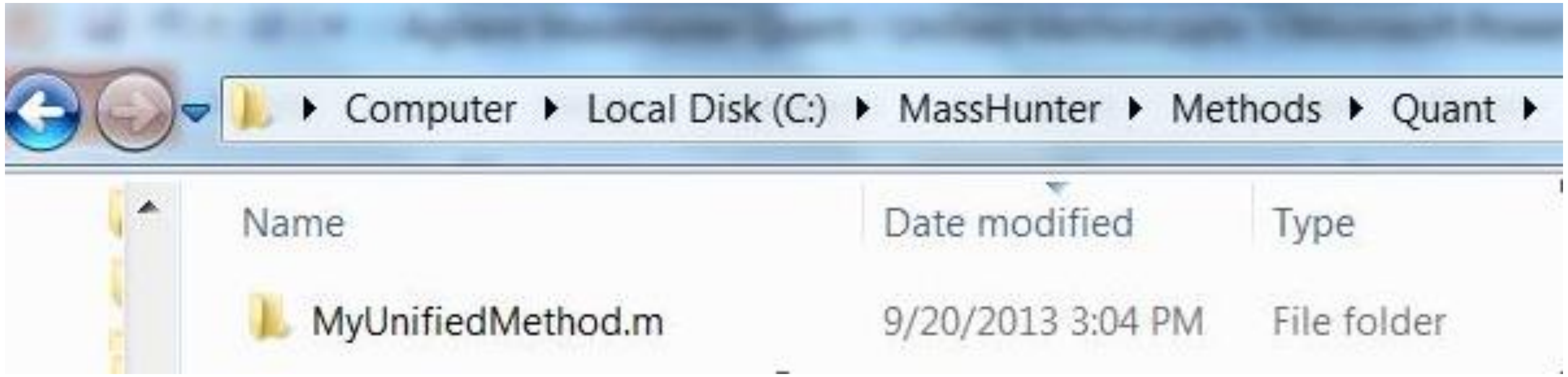
Collect
Data

Unified Method

One location, one name

- Defines acquisition method
- Defines analysis method
- Defines report method

Allows granular control over analysis and reporting by sample



Computer ▸ Local Disk (C:) ▸ MassHunter ▸ Methods ▸ Quant ▸

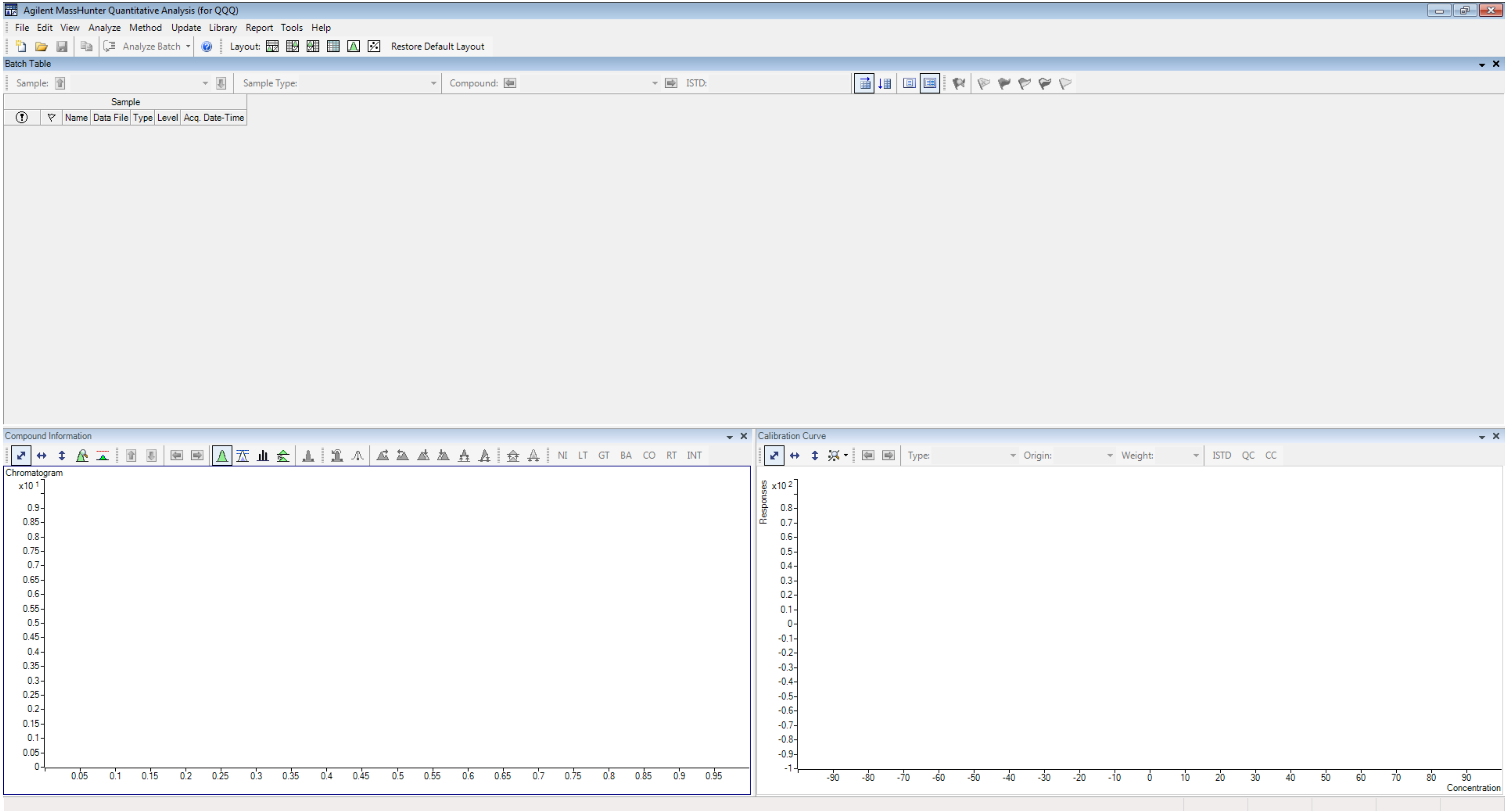
Name	Date modified	Type
MyUnifiedMethod.m	9/20/2013 3:04 PM	File folder

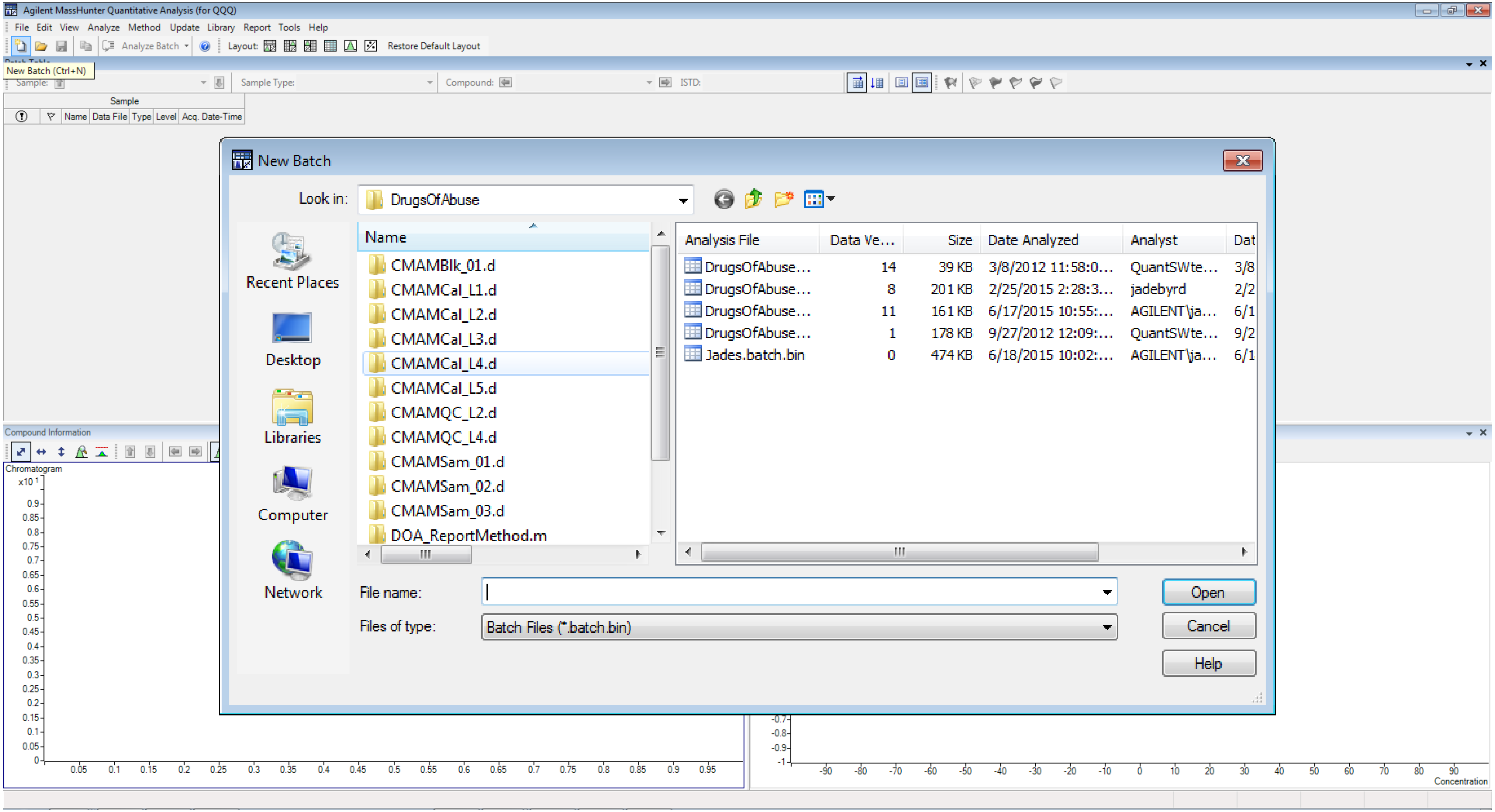
MassHunter Quantative Analysis Workflow

Import
or
Manually Create
Sample List

Collect
Data

Review-
by-
Exception


Agilent MassHunter Quantitative Analysis (for QQQ)
File Edit View Analyze Method Update Library Report Tools Help
Analyze Batch
Layout:
Restore Default Layout
Batch Table
Sample:
Sample Type:
Compound:
ISTD:
Sample
Name
Data File
Type
Level
Acq. Date-Time
Compound Information
NI LT GT BA CO RT INT
Chromatogram
x10 1
0.9
0.85
0.8
0.75
0.7
0.65
0.6
0.55
0.5
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
0.05 0.1 0.15 0.2 0.25 0.3 0.35 0.4 0.45 0.5 0.55 0.6 0.65 0.7 0.75 0.8 0.85 0.9 0.95
Calibration Curve
Type:
Origin:
Weight:
ISTD QC CC
Responses
x10 2
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
-0.4
-0.5
-0.6
-0.7
-0.8
-0.9
-1
-90 -80 -70 -60 -50 -40 -30 -20 -10 0 10 20 30 40 50 60 70 80 90
Concentration



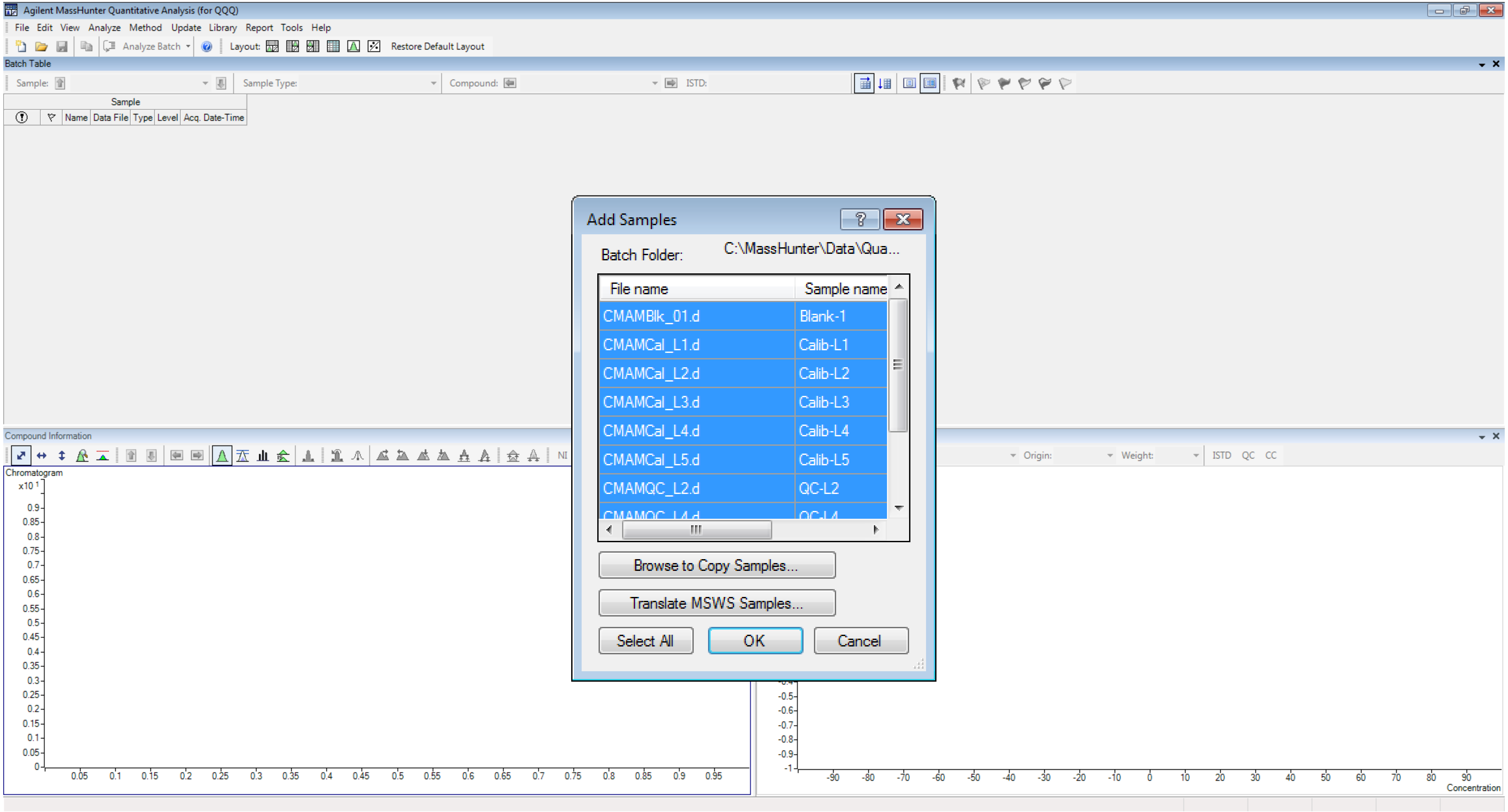
Look in: DrugsOfAbuse

Name
CMAMBlk_01.d
CMAMCal_L1.d
CMAMCal_L2.d
CMAMCal_L3.d
CMAMCal_L4.d
CMAMCal_L5.d
CMAMQC_L2.d
CMAMQC_L4.d
CMAMSam_01.d
CMAMSam_02.d
CMAMSam_03.d
DOA_ReportMethod.m

Analysis File	Data Ve...	Size	Date Analyzed	Analyst	Dat
DrugsOfAbuse...	14	39 KB	3/8/2012 11:58:0...	QuantSWte...	3/8
DrugsOfAbuse...	8	201 KB	2/25/2015 2:28:3...	jadebyrd	2/2
DrugsOfAbuse...	11	161 KB	6/17/2015 10:55:...	AGILENT\ja...	6/1
DrugsOfAbuse...	1	178 KB	9/27/2012 12:09:...	QuantSWte...	9/2
Jades.batch.bin	0	474 KB	6/18/2015 10:02:...	AGILENT\ja...	6/1

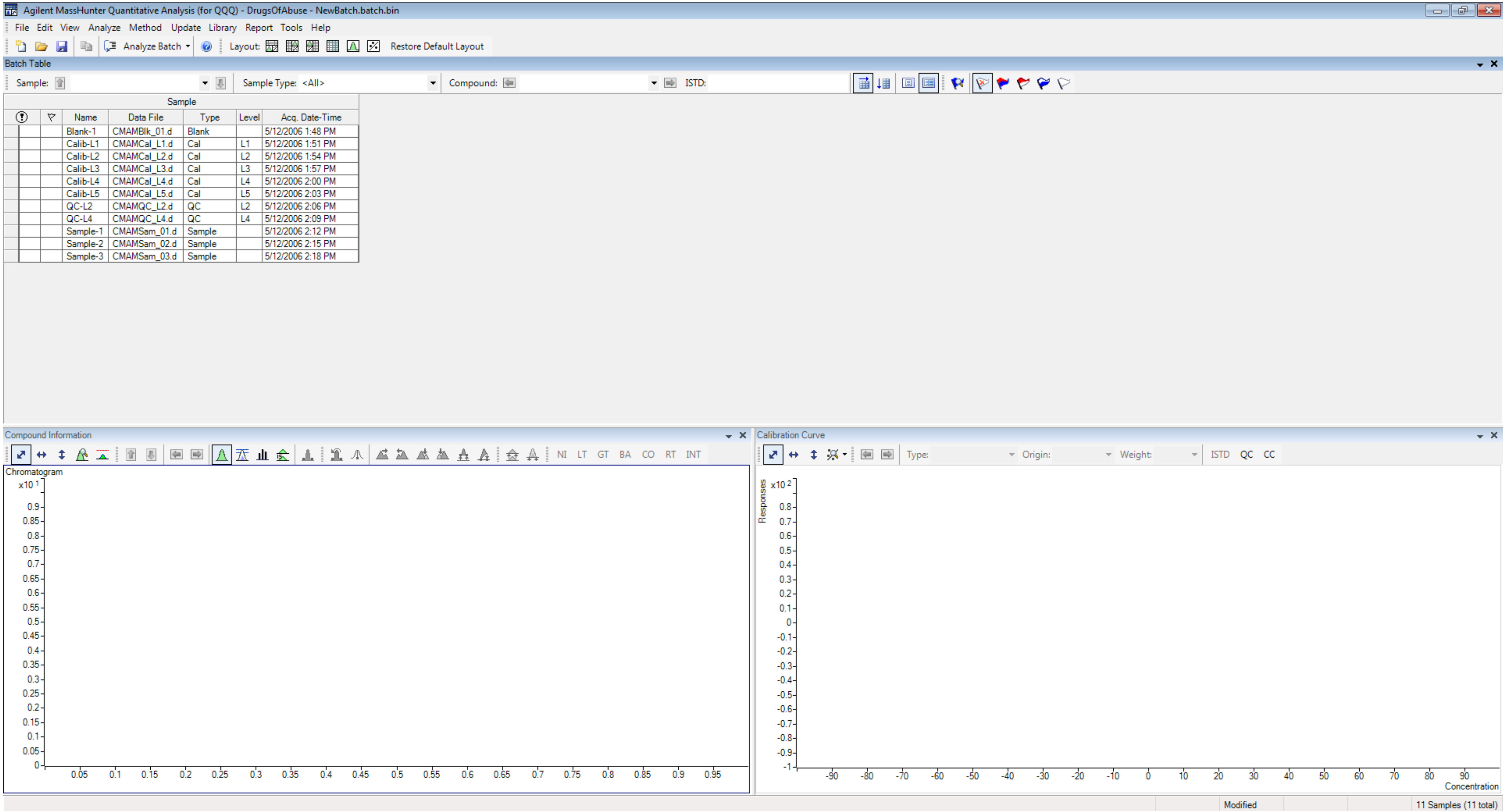
File name:

Files of type: Batch Files (*.batch.bin)

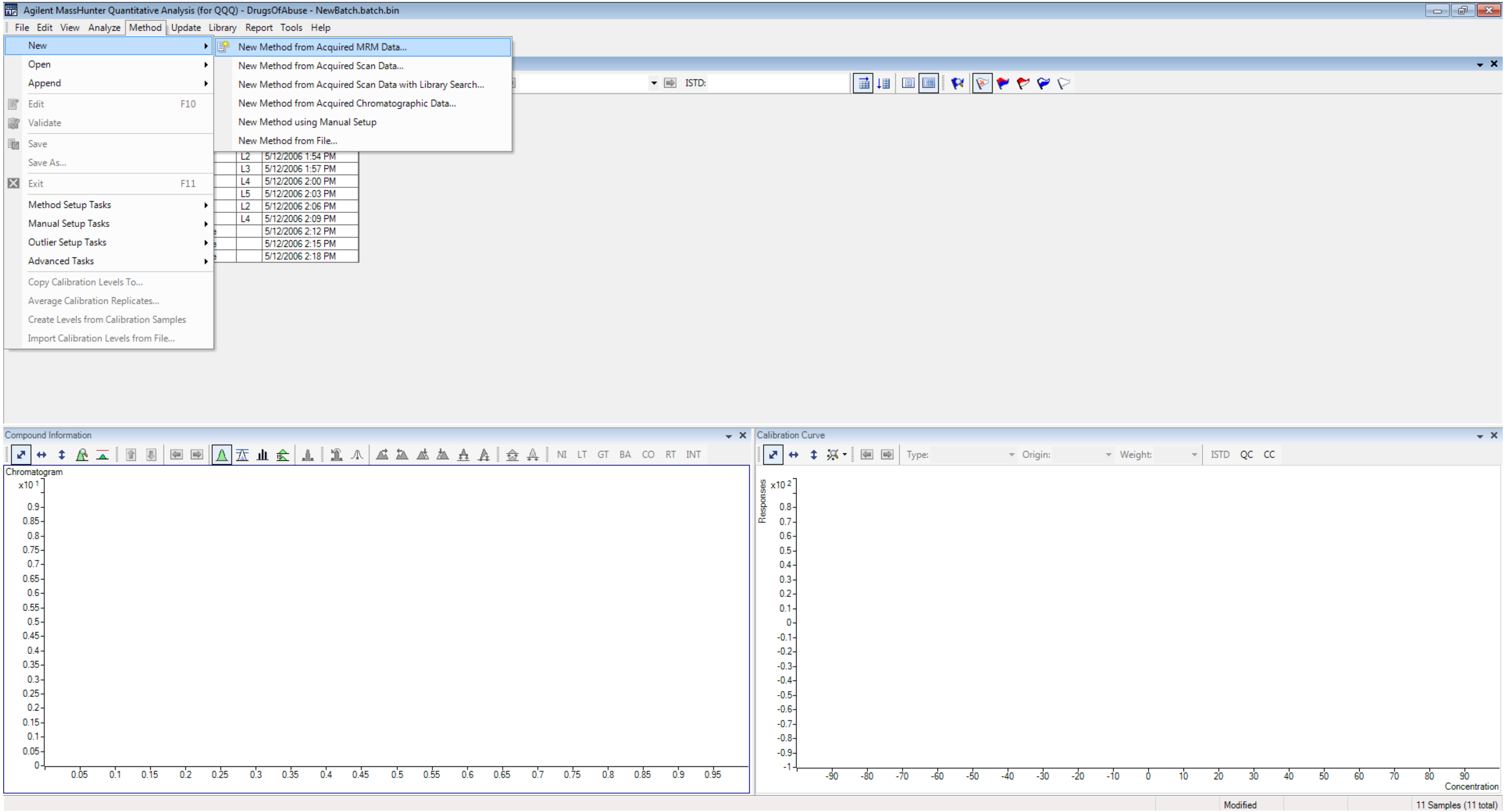


Batch Folder: C:\MassHunter\Data\Qua...

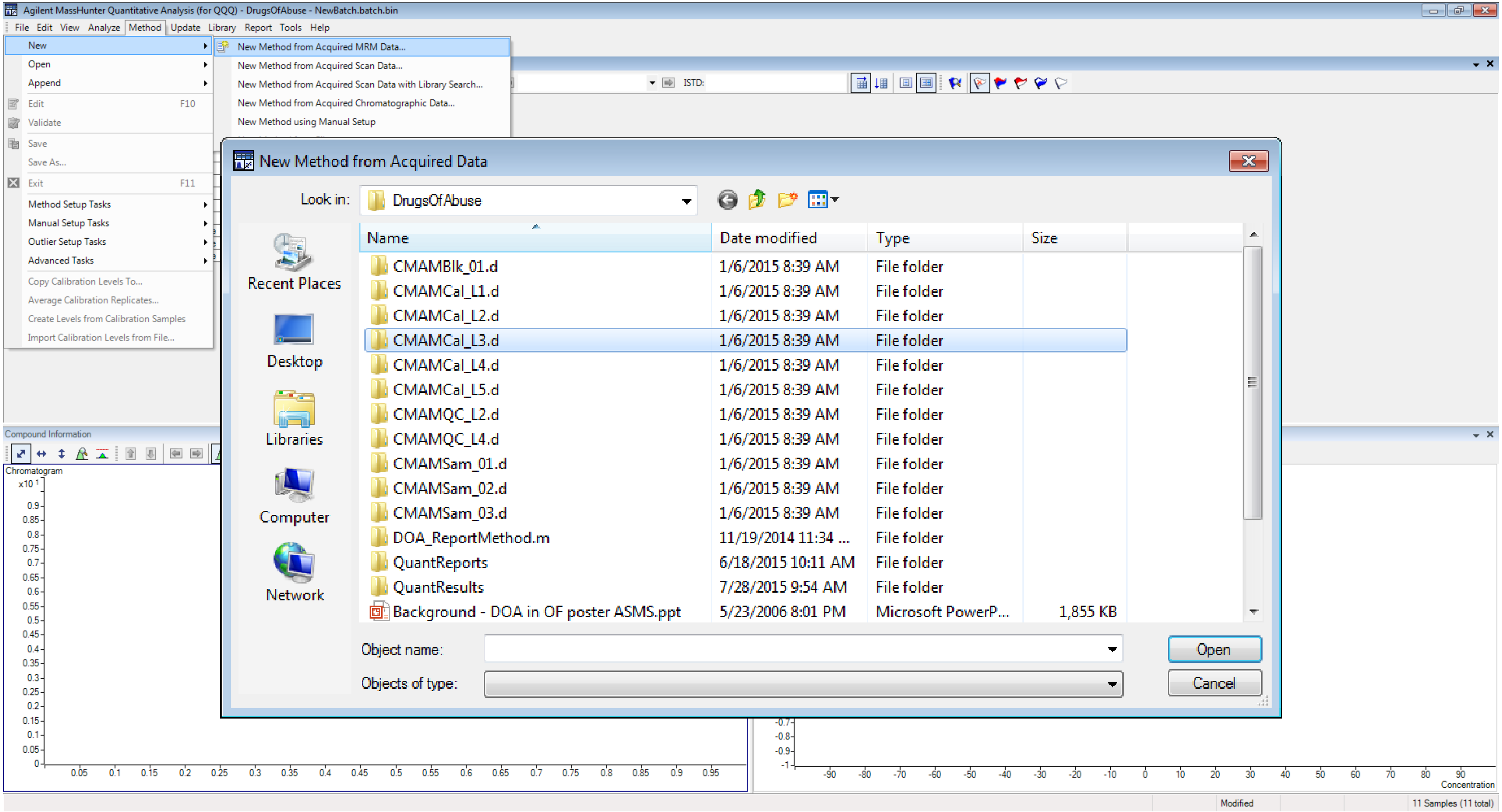
File name	Sample name
CMAMBlk_01.d	Blank-1
CMAMCal_L1.d	Calib-L1
CMAMCal_L2.d	Calib-L2
CMAMCal_L3.d	Calib-L3
CMAMCal_L4.d	Calib-L4
CMAMCal_L5.d	Calib-L5
CMAMQC_L2.d	QC-L2
CMAMQC_L4.d	QC-L4



		Sample				
ⓘ	▽	Name	Data File	Type	Level	Acq. Date-Time
		Blank-1	CMAMBlk_01.d	Blank		5/12/2006 1:48 PM
		Calib-L1	CMAMCal_L1.d	Cal	L1	5/12/2006 1:51 PM
		Calib-L2	CMAMCal_L2.d	Cal	L2	5/12/2006 1:54 PM
		Calib-L3	CMAMCal_L3.d	Cal	L3	5/12/2006 1:57 PM
		Calib-L4	CMAMCal_L4.d	Cal	L4	5/12/2006 2:00 PM
		Calib-L5	CMAMCal_L5.d	Cal	L5	5/12/2006 2:03 PM
		QC-L2	CMAMQC_L2.d	QC	L2	5/12/2006 2:06 PM
		QC-L4	CMAMQC_L4.d	QC	L4	5/12/2006 2:09 PM
		Sample-1	CMAMSam_01.d	Sample		5/12/2006 2:12 PM
		Sample-2	CMAMSam_02.d	Sample		5/12/2006 2:15 PM
		Sample-3	CMAMSam_03.d	Sample		5/12/2006 2:18 PM



L2	5/12/2006 1:54 PM
L3	5/12/2006 1:57 PM
L4	5/12/2006 2:00 PM
L5	5/12/2006 2:03 PM
L2	5/12/2006 2:06 PM
L4	5/12/2006 2:09 PM
	5/12/2006 2:12 PM
	5/12/2006 2:15 PM
	5/12/2006 2:18 PM



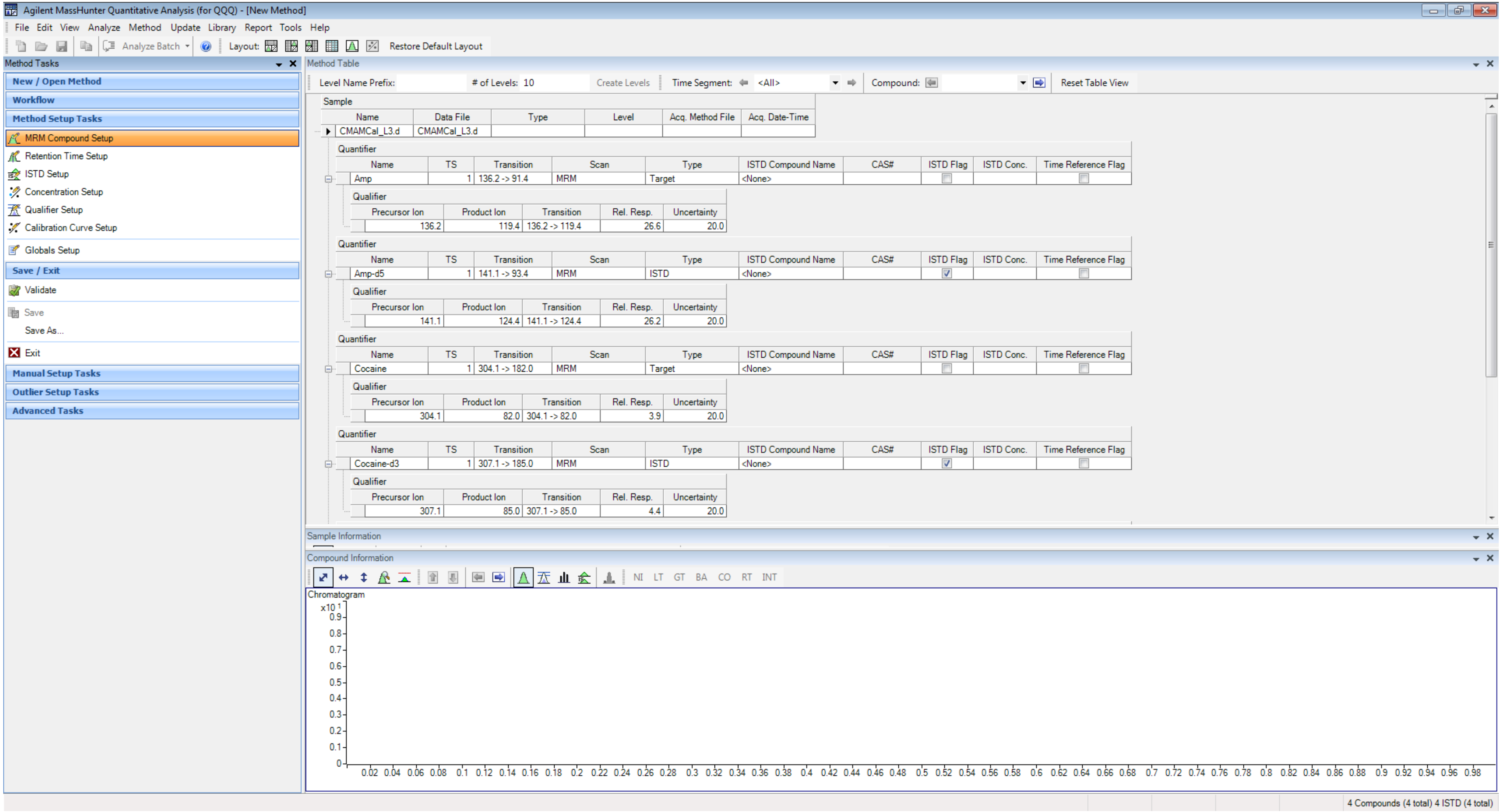
New Method from Acquired Data

Look in: DrugsOfAbuse

Name	Date modified	Type	Size
CMAMBlk_01.d	1/6/2015 8:39 AM	File folder	
CMAMCal_L1.d	1/6/2015 8:39 AM	File folder	
CMAMCal_L2.d	1/6/2015 8:39 AM	File folder	
CMAMCal_L3.d	1/6/2015 8:39 AM	File folder	
CMAMCal_L4.d	1/6/2015 8:39 AM	File folder	
CMAMCal_L5.d	1/6/2015 8:39 AM	File folder	
CMAMQC_L2.d	1/6/2015 8:39 AM	File folder	
CMAMQC_L4.d	1/6/2015 8:39 AM	File folder	
CMAMSam_01.d	1/6/2015 8:39 AM	File folder	
CMAMSam_02.d	1/6/2015 8:39 AM	File folder	
CMAMSam_03.d	1/6/2015 8:39 AM	File folder	
DOA_ReportMethod.m	11/19/2014 11:34 ...	File folder	
QuantReports	6/18/2015 10:11 AM	File folder	
QuantResults	7/28/2015 9:54 AM	File folder	
Background - DOA in OF poster ASMS.ppt	5/23/2006 8:01 PM	Microsoft PowerP...	1,855 KB

Object name:

Objects of type:



Level Name Prefix: # of Levels: 10

Time Segment: <All>

Compound:

Sample

Name	Data File	Type	Level	Acq. Method File	Acq. Date-Time
CMAMCal_L3.d	CMAMCal_L3.d				

Quantifier

Name	TS	Transition	Scan	Type	ISTD Compound Name	CAS#	ISTD Flag	ISTD Conc.	Time Reference Flag
Amp	1	136.2 -> 91.4	MRM	Target	<None>		☐		☐

Qualifier

Precursor Ion	Product Ion	Transition	Rel. Resp.	Uncertainty
136.2	119.4	136.2 -> 119.4	26.6	20.0

Quantifier

Name	TS	Transition	Scan	Type	ISTD Compound Name	CAS#	ISTD Flag	ISTD Conc.	Time Reference Flag
Amp-d5	1	141.1 -> 93.4	MRM	ISTD	<None>		☑		☐

Qualifier

Precursor Ion	Product Ion	Transition	Rel. Resp.	Uncertainty
141.1	124.4	141.1 -> 124.4	26.2	20.0

Quantifier

Name	TS	Transition	Scan	Type	ISTD Compound Name	CAS#	ISTD Flag	ISTD Conc.	Time Reference Flag
Cocaine	1	304.1 -> 182.0	MRM	Target	<None>		☐		☐

Qualifier

Precursor Ion	Product Ion	Transition	Rel. Resp.	Uncertainty
304.1	82.0	304.1 -> 82.0	3.9	20.0

Quantifier

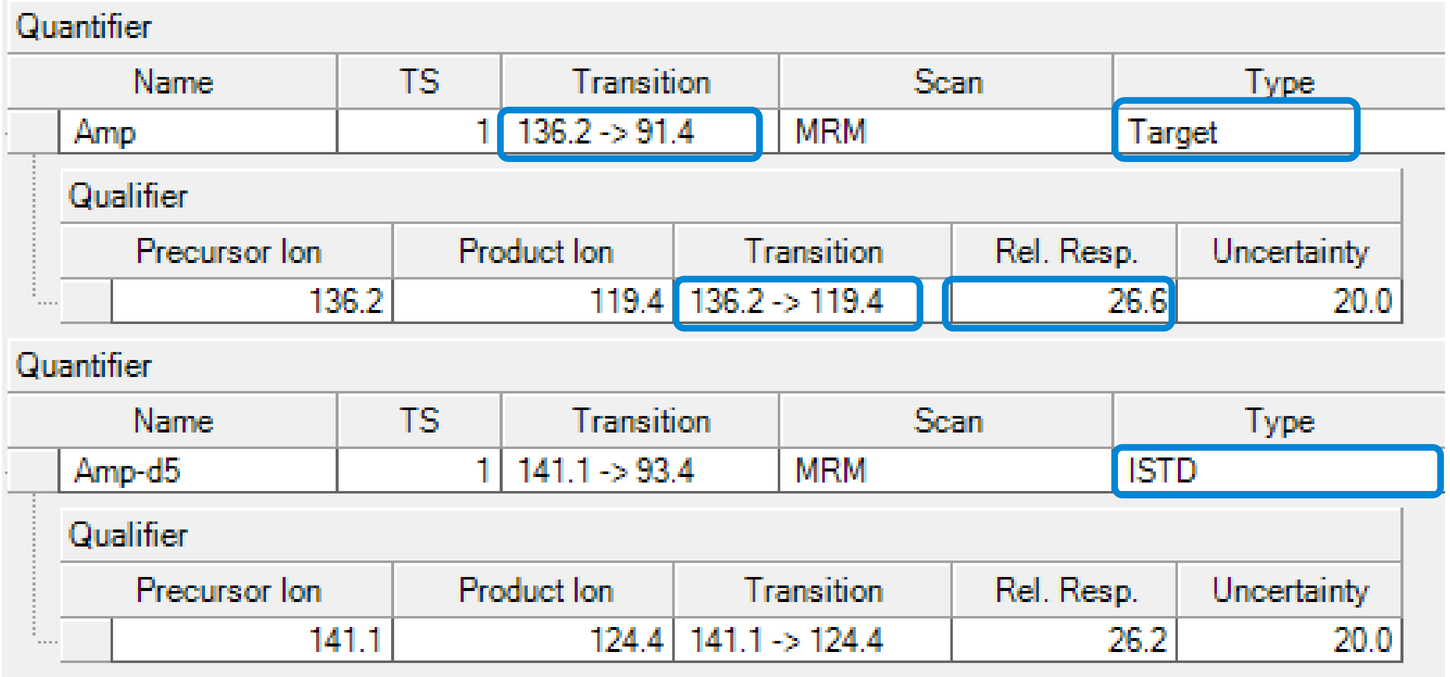
Name	TS	Transition	Scan	Type	ISTD Compound Name	CAS#	ISTD Flag	ISTD Conc.	Time Reference Flag
Cocaine-d3	1	307.1 -> 185.0	MRM	ISTD	<None>		☑		☐

Qualifier

Precursor Ion	Product Ion	Transition	Rel. Resp.	Uncertainty
307.1	85.0	307.1 -> 85.0	4.4	20.0

4 Compounds (4 total) 4 ISTD (4 total)

Target, Internal Standard and Qualifier Ion Ratios learned from the Data



Quantifier

Name	TS	Transition	Scan	Type
Amp	1	136.2 -> 91.4	MRM	Target

Qualifier

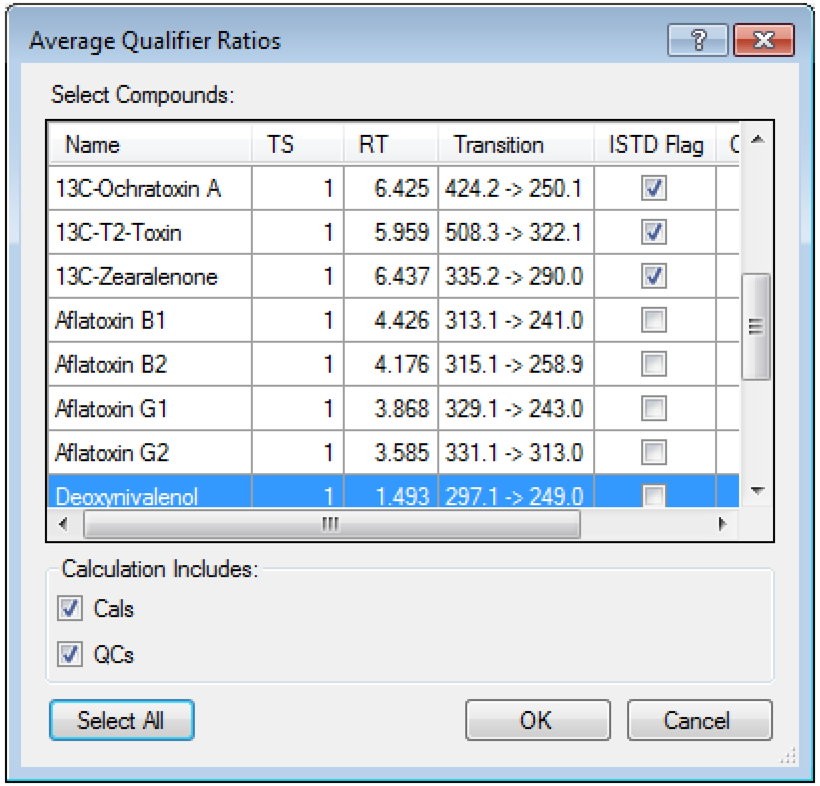
Precursor Ion	Product Ion	Transition	Rel. Resp.	Uncertainty
136.2	119.4	136.2 -> 119.4	26.6	20.0

Quantifier

Name	TS	Transition	Scan	Type
Amp-d5	1	141.1 -> 93.4	MRM	ISTD

Qualifier

Precursor Ion	Product Ion	Transition	Rel. Resp.	Uncertainty
141.1	124.4	141.1 -> 124.4	26.2	20.0



Average Qualifier Ratios

Select Compounds:

Name	TS	RT	Transition	ISTD Flag
13C-Ochratoxin A	1	6.425	424.2 -> 250.1	☑
13C-T2-Toxin	1	5.959	508.3 -> 322.1	☑
13C-Zearalenone	1	6.437	335.2 -> 290.0	☑
Aflatoxin B1	1	4.426	313.1 -> 241.0	☐
Aflatoxin B2	1	4.176	315.1 -> 258.9	☐
Aflatoxin G1	1	3.868	329.1 -> 243.0	☐
Aflatoxin G2	1	3.585	331.1 -> 313.0	☐
Deoxynivalenol	1	1.493	297.1 -> 249.0	☐

Calculation Includes:

☑ Cals

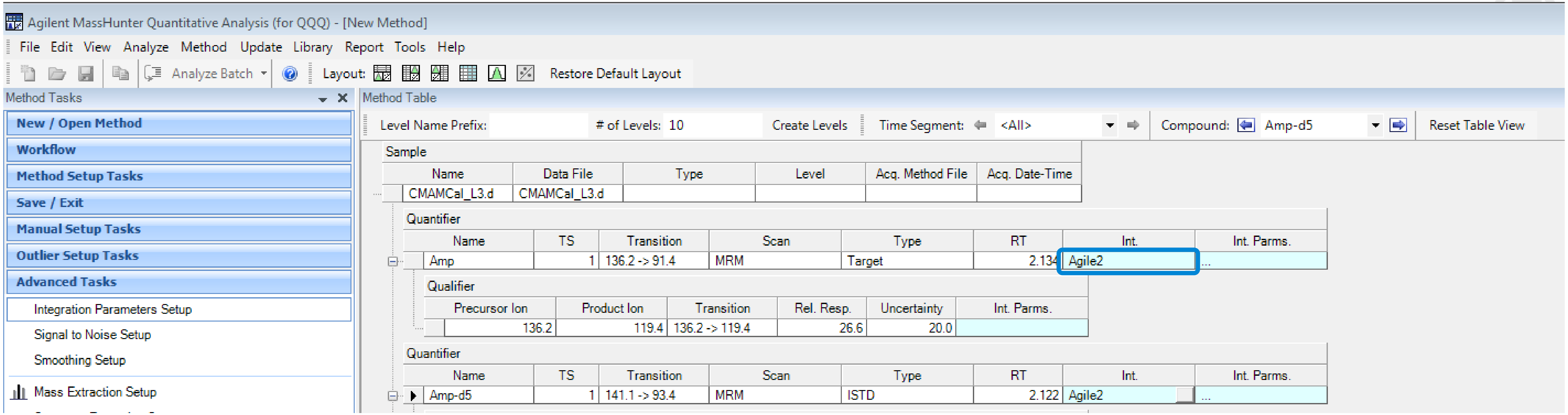
☑ QCs

New in B.07.00 – SIM from GC/MSD works the same as MRM

Available for MSD, QQQ, TOF, and Q-TOF

Peak Detection

Each peak can be configured to use 1 of 5 peak detection algorithms



Level Name Prefix: # of Levels: 10 Time Segment: <All> Compound: Amp-d5

Sample

Name	Data File	Type	Level	Acq. Method File	Acq. Date-Time
CMAMCal_L3.d	CMAMCal_L3.d				

Quantifier

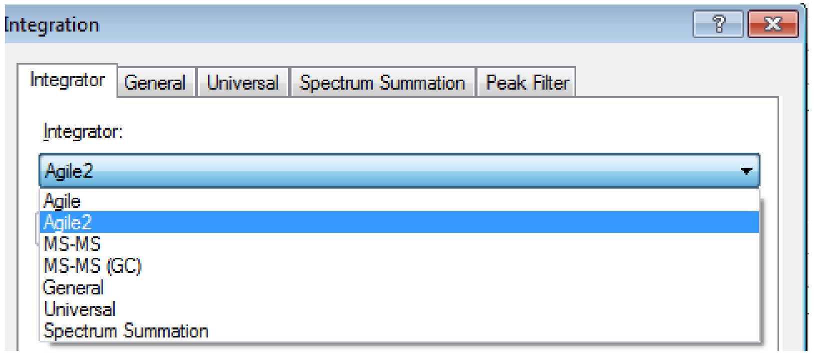
Name	TS	Transition	Scan	Type	RT	Int.	Int. Parms.
Amp	1	136.2 -> 91.4	MRM	Target	2.134	Agile2	...

Qualifier

Precursor Ion	Product Ion	Transition	Rel. Resp.	Uncertainty	Int. Parms.
136.2	119.4	136.2 -> 119.4	26.6	20.0	

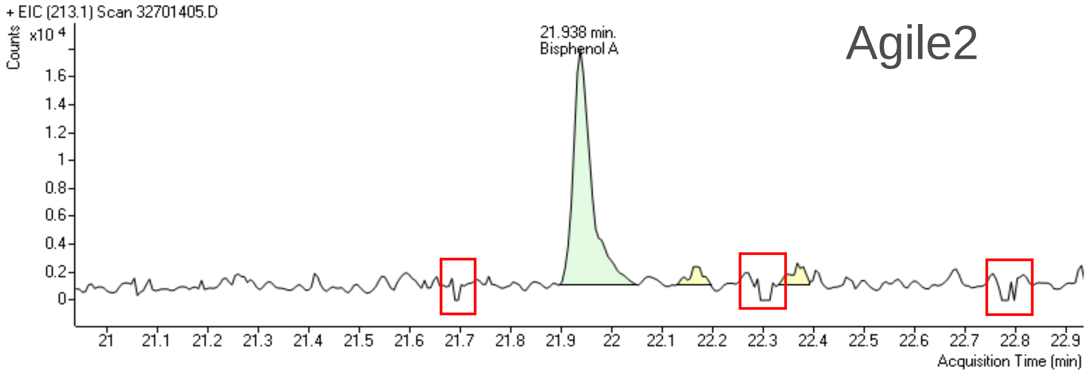
Quantifier

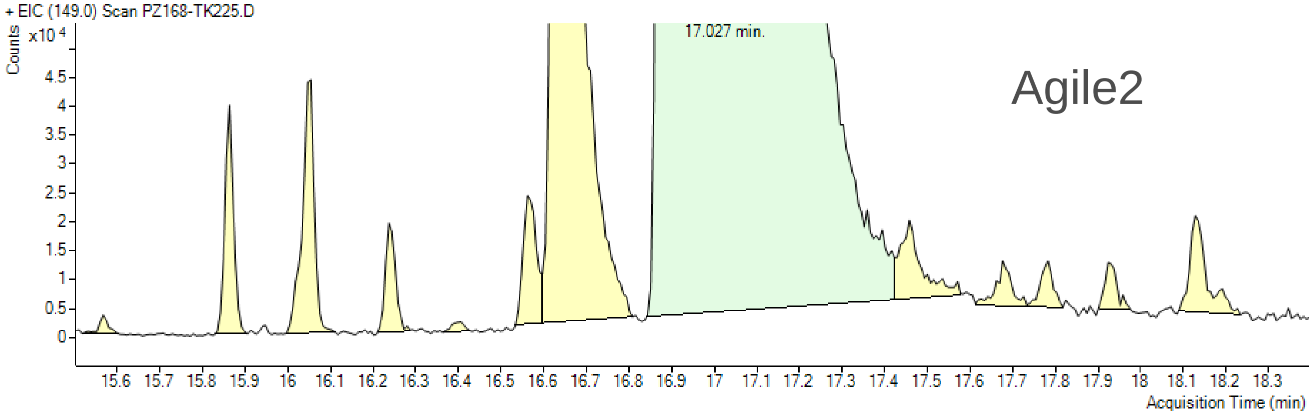
Name	TS	Transition	Scan	Type	RT	Int.	Int. Parms.
Amp-d5	1	141.1 -> 93.4	MRM	ISTD	2.122	Agile2	...

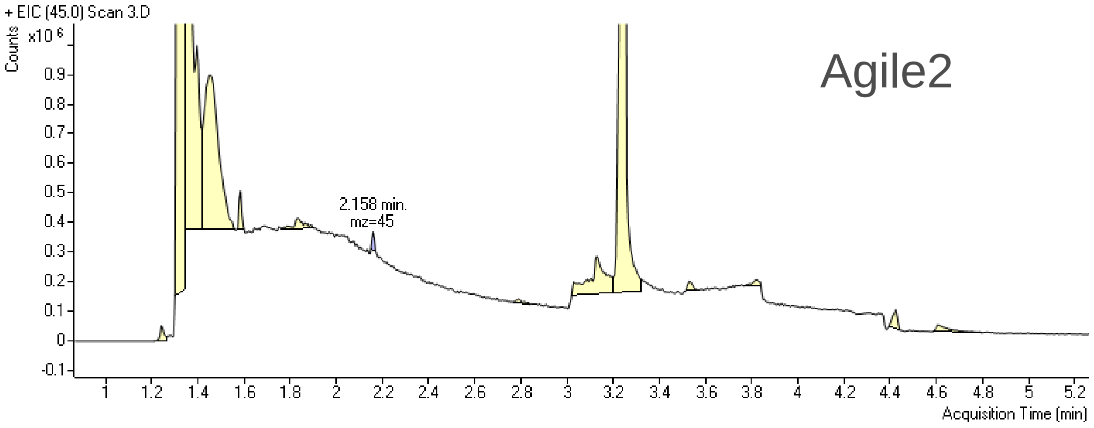


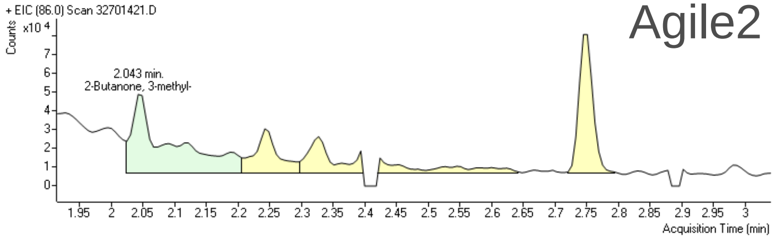
Integrator: Agile2

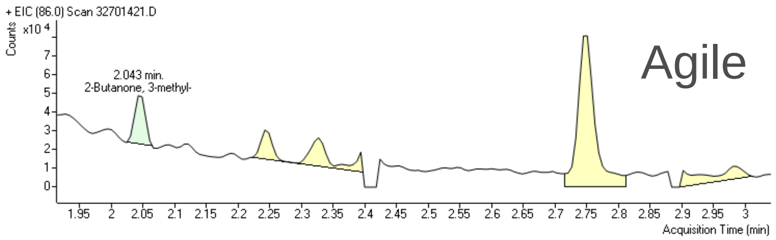
Agile and Agile2 – parameter-less integrators



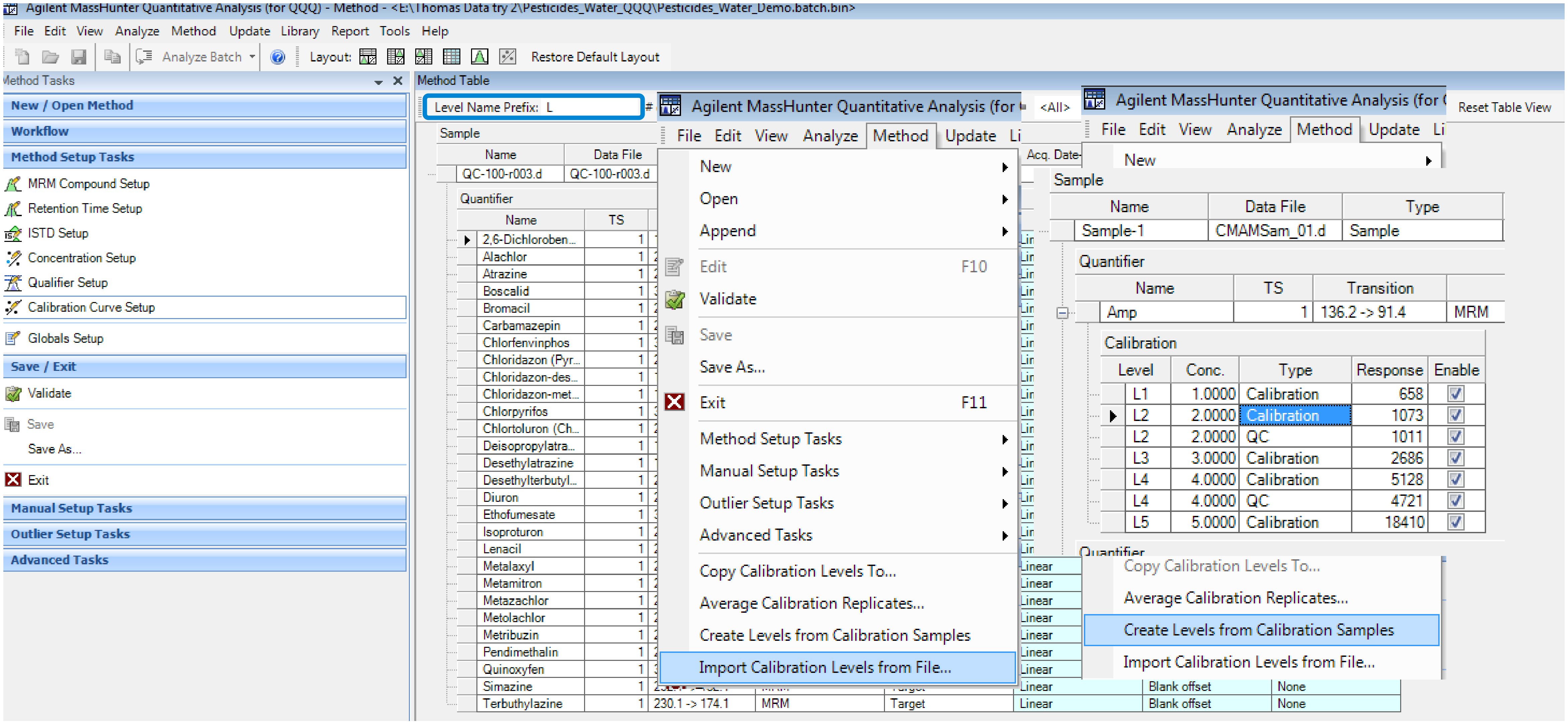








Building the Calibration Table



Sample

Name	Data File	Type
Sample-1	CMAMSam_01.d	Sample

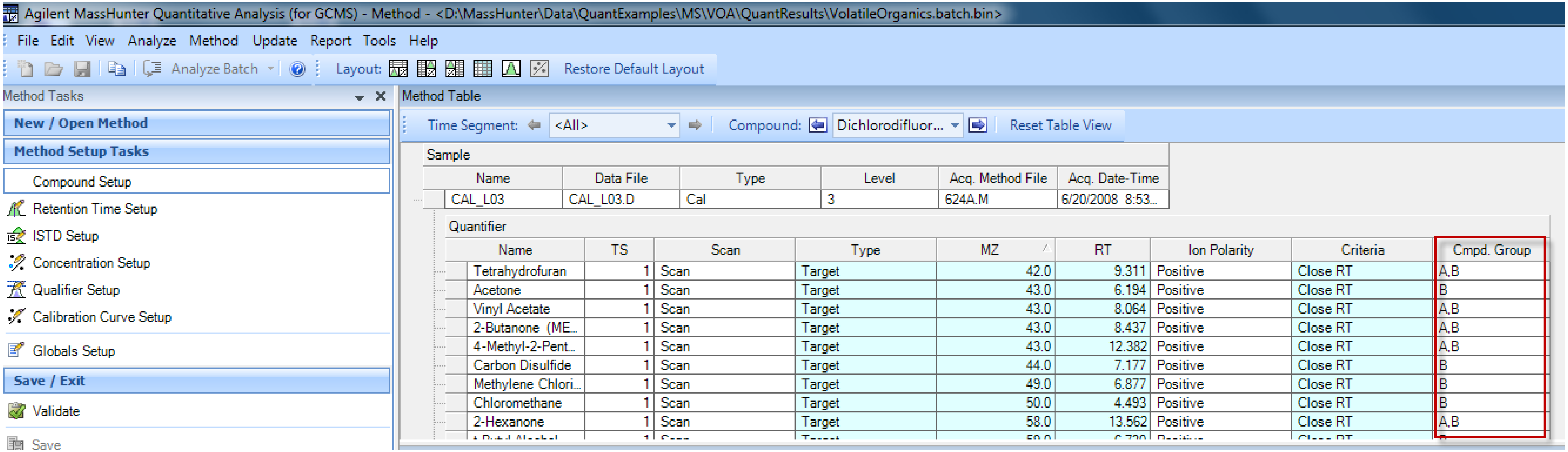
Quantifier

Name	TS	Transition	
Amp	1	136.2 -> 91.4	MRM

Calibration

Level	Conc.	Type	Response	Enable
L1	1.0000	Calibration	658	☑
L2	2.0000	Calibration	1073	☑
L2	2.0000	QC	1011	☑
L3	3.0000	Calibration	2686	☑
L4	4.0000	Calibration	5128	☑
L4	4.0000	QC	4721	☑
L5	5.0000	Calibration	18410	☑

Compound Group Sample & Compound based Review/Report



Time Segment: <All>

Compound: Dichlorodifluor...

Sample

Name	Data File	Type	Level	Acq. Method File	Acq. Date-Time
CAL_L03	CAL_L03.D	Cal	3	624A.M	6/20/2008 8:53...

Quantifier

Name	TS	Scan	Type	MZ	RT	Ion Polarity	Criteria	Cmpd. Group
Tetrahydrofuran	1	Scan	Target	42.0	9.311	Positive	Close RT	A,B
Acetone	1	Scan	Target	43.0	6.194	Positive	Close RT	B
Vinyl Acetate	1	Scan	Target	43.0	8.064	Positive	Close RT	A,B
2-Butanone (ME...	1	Scan	Target	43.0	8.437	Positive	Close RT	A,B
4-Methyl-2-Pent...	1	Scan	Target	43.0	12.382	Positive	Close RT	A,B
Carbon Disulfide	1	Scan	Target	44.0	7.177	Positive	Close RT	B
Methylene Chlori...	1	Scan	Target	49.0	6.877	Positive	Close RT	B
Chloromethane	1	Scan	Target	50.0	4.493	Positive	Close RT	B
2-Hexanone	1	Scan	Target	58.0	13.562	Positive	Close RT	A,B

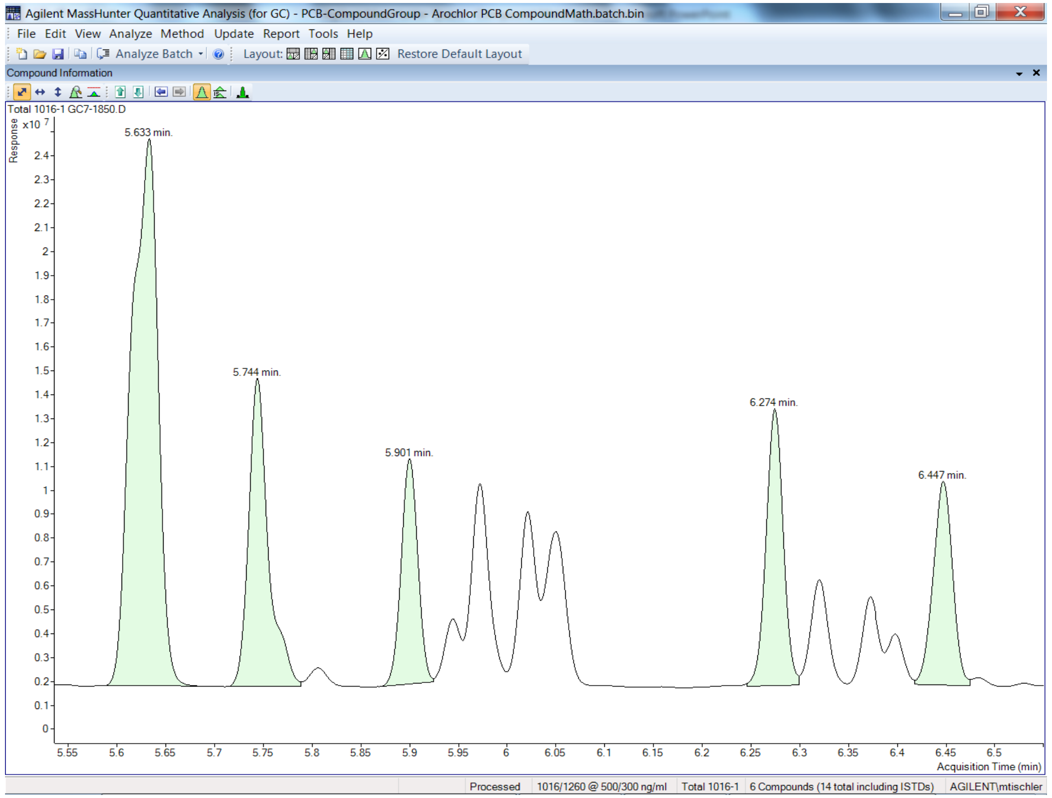
Useful when there is one analysis method but wish to review and report different sets of the compound list based on individual samples

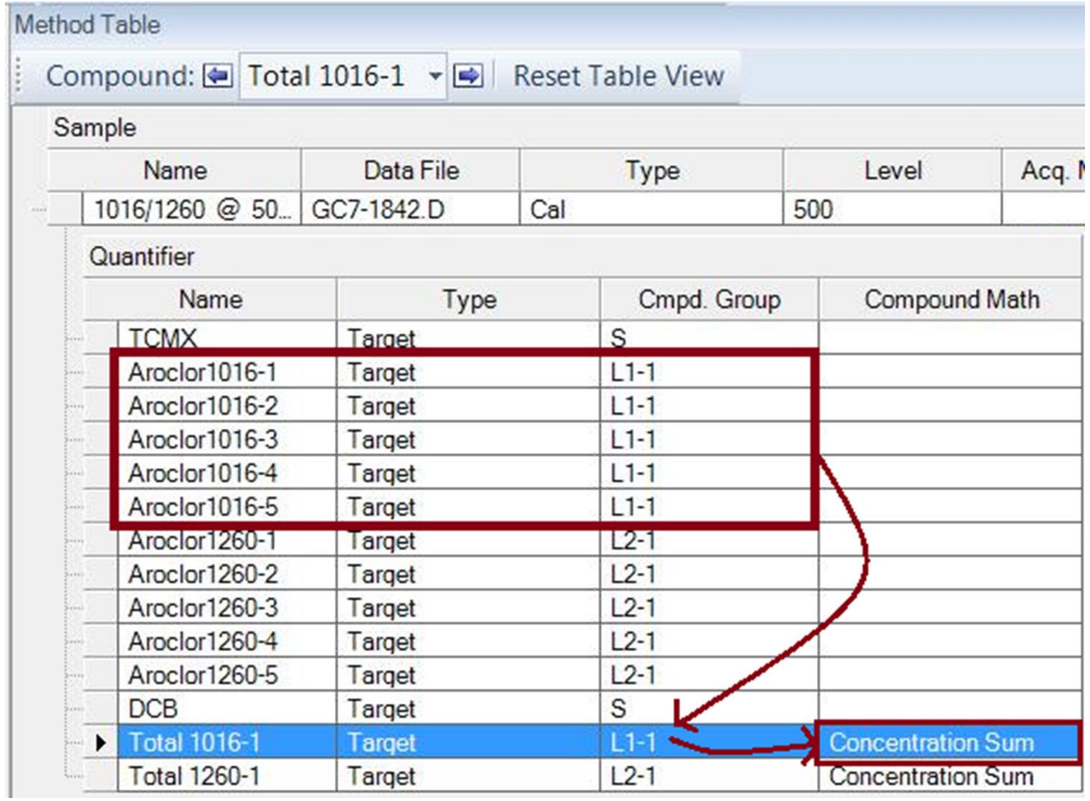
Also used for StreamSelect (2 or 4 streams)

Compound Math: group peaks for calibration and quantitation

Five peaks representing

Aroclor PCBs mixture





Compound: Total 1016-1

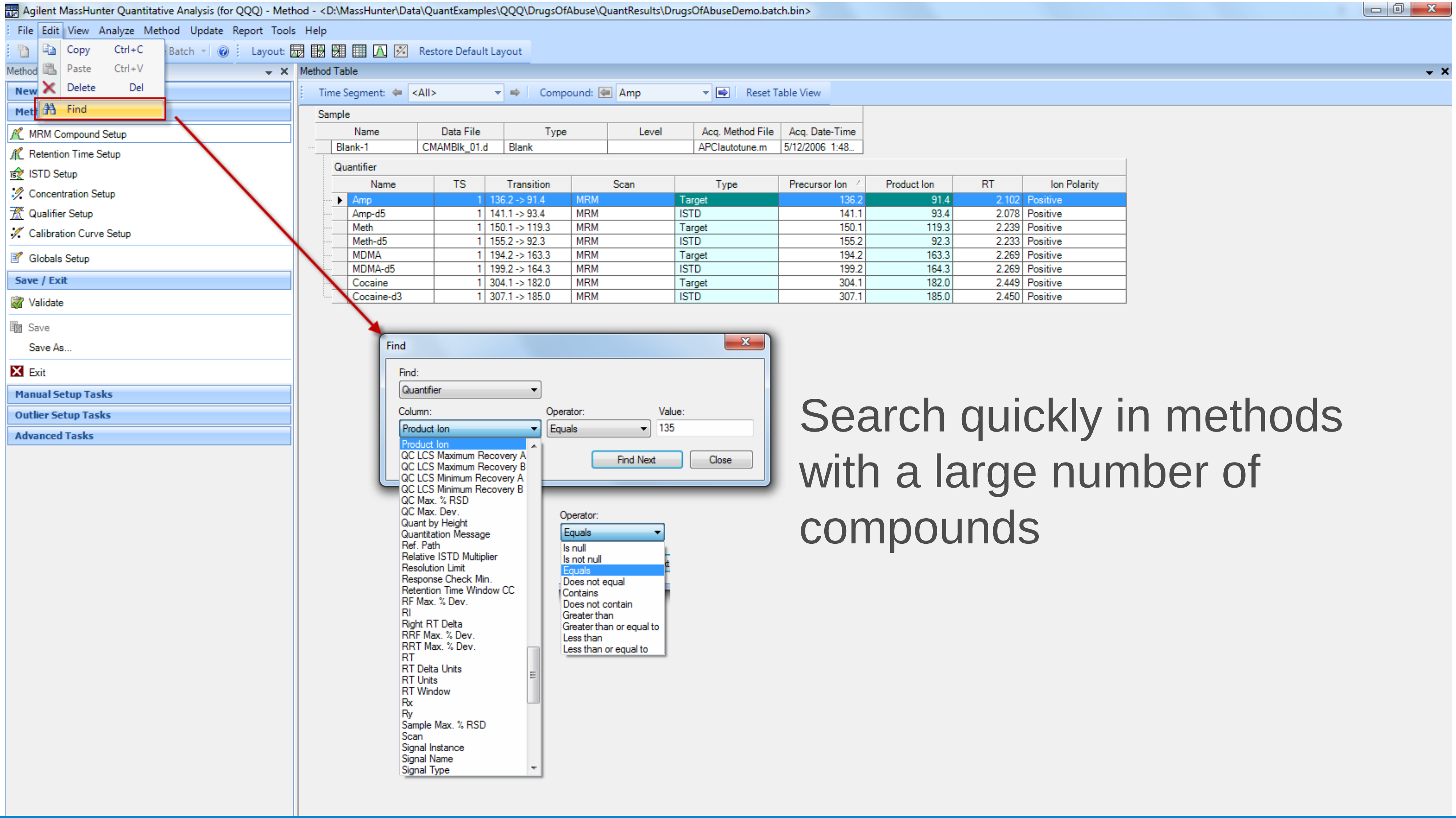
Sample

Name	Data File	Type	Level	Acq.
1016/1260 @ 50...	GC7-1842.D	Cal	500	

Quantifier

Name	Type	Cmpd. Group	Compound Math
TCMX	Target	S	
Aroclor1016-1	Target	L1-1	
Aroclor1016-2	Target	L1-1	
Aroclor1016-3	Target	L1-1	
Aroclor1016-4	Target	L1-1	
Aroclor1016-5	Target	L1-1	
Aroclor1260-1	Target	L2-1	
Aroclor1260-2	Target	L2-1	
Aroclor1260-3	Target	L2-1	
Aroclor1260-4	Target	L2-1	
Aroclor1260-5	Target	L2-1	
DCB	Target	S	
Total 1016-1	Target	L1-1	Concentration Sum
Total 1260-1	Target	L2-1	Concentration Sum

New Find Feature in Method Editor



Agilent MassHunter Quantitative Analysis (for QQQ) - Method - <D:\MassHunter\Data\QuantExamples\QQQ\DrugsOfAbuse\QuantResults\DrugsOfAbuseDemo.batch.bin>

Method Table

Time Segment: <All>

Compound: Amp

Sample

Name	Data File	Type	Level	Acq. Method File	Acq. Date-Time
Blank-1	CMAMBlk_01.d	Blank		APCIautotune.m	5/12/2006 1:48...

Quantifier

Name	TS	Transition	Scan	Type	Precursor Ion	Product Ion	RT	Ion Polarity
Amp	1	136.2 -> 91.4	MRM	Target	136.2	91.4	2.102	Positive
Amp-d5	1	141.1 -> 93.4	MRM	ISTD	141.1	93.4	2.078	Positive
Meth	1	150.1 -> 119.3	MRM	Target	150.1	119.3	2.239	Positive
Meth-d5	1	155.2 -> 92.3	MRM	ISTD	155.2	92.3	2.233	Positive
MDMA	1	194.2 -> 163.3	MRM	Target	194.2	163.3	2.269	Positive
MDMA-d5	1	199.2 -> 164.3	MRM	ISTD	199.2	164.3	2.269	Positive
Cocaine	1	304.1 -> 182.0	MRM	Target	304.1	182.0	2.449	Positive
Cocaine-d3	1	307.1 -> 185.0	MRM	ISTD	307.1	185.0	2.450	Positive

Find

Find: Quantifier

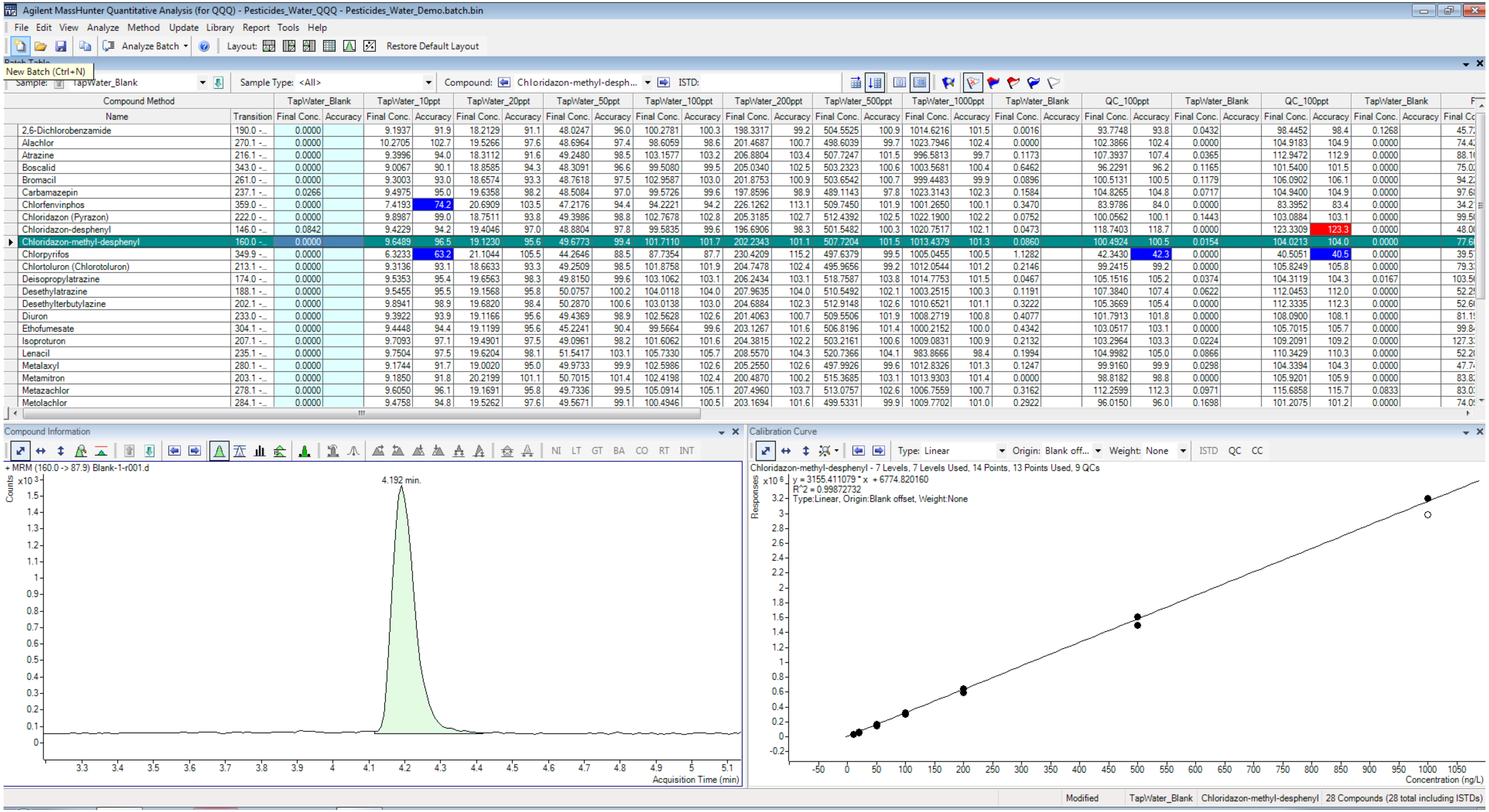
Column: Product Ion

Operator: Equals

Value: 135

Search quickly in methods with a large number of compounds

After applying the Analysis Method



Agilent MassHunter Quantitative Analysis (for QQQ) - Pesticides_Water_QQQ - Pesticides_Water_Demo.batch.bin

Sample: TapWater_Blank

Sample Type: <All>

Compound: Chloridazon-methyl-desph...

ISTD:

Compound Method		TapWater_Blank		TapWater_10ppt		TapWater_20ppt		TapWater_50ppt		TapWater_100ppt		TapWater_200ppt		TapWater_500ppt		TapWater_1000ppt		TapWater_Blank		QC_100ppt		TapWater_Blank		QC_100ppt		TapWater_Blank		F
Name	Transition	Final Conc.	Accuracy	Final Conc.	Accuracy	Final Conc.	Accuracy	Final Conc.	Accuracy	Final Conc.	Accuracy	Final Conc.	Accuracy	Final Conc.	Accuracy	Final Conc.	Accuracy	Final Conc.	Accuracy	Final Conc.	Accuracy	Final Conc.	Accuracy	Final Conc.	Accuracy	Final Conc.	Accuracy	Final Conc.	Accuracy	Final Co
2,6-Dichlorobenzamide	190.0 -...	0.0000		9.1937	91.9	18.2129	91.1	48.0247	96.0	100.2781	100.3	198.3317	99.2	504.5525	100.9	1014.6216	101.5	0.0016		93.7748	93.8	0.0432		98.4452	98.4	0.1268		45.7
Alachlor	270.1 -...	0.0000		10.2705	102.7	19.5266	97.6	48.6964	97.4	98.6059	98.6	201.4687	100.7	498.6039	99.7	1023.7946	102.4	0.0000		102.3866	102.4	0.0000		104.9183	104.9	0.0000		74.4
Atrazine	216.1 -...	0.0000		9.3996	94.0	18.3112	91.6	49.2480	98.5	103.1577	103.2	206.8804	103.4	507.7247	101.5	996.5813	99.7	0.1173		107.3937	107.4	0.0365		112.9472	112.9	0.0000		88.1
Boscalid	343.0 -...	0.0000		9.0067	90.1	18.8585	94.3	48.3091	96.6	99.5080	99.5	205.0340	102.5	503.2323	100.6	1003.5681	100.4	0.6462		96.2291	96.2	0.1165		101.5400	101.5	0.0000		75.0
Bromacil	261.0 -...	0.0000		9.3003	93.0	18.6574	93.3	48.7618	97.5	102.9587	103.0	201.8753	100.9	503.6542	100.7	999.4483	99.9	0.0896		100.5131	100.5	0.1179		106.0902	106.1	0.0000		94.2
Carbamazepin	237.1 -...	0.0266		9.4975	95.0	19.6358	98.2	48.5084	97.0	99.5726	99.6	197.8596	98.9	489.1143	97.8	1023.3143	102.3	0.1584		104.8265	104.8	0.0717		104.9400	104.9	0.0000		97.6
Chlorfenvinphos	359.0 -...	0.0000		7.4193	74.2	20.6909	103.5	47.2176	94.4	94.2221	94.2	226.1262	113.1	509.7450	101.9	1001.2650	100.1	0.3470		83.9786	84.0	0.0000		83.3952	83.4	0.0000		34.2
Chloridazon (Pyrazon)	222.0 -...	0.0000		9.8987	99.0	18.7511	93.8	49.3986	98.8	102.7678	102.8	205.3185	102.7	512.4392	102.5	1022.1900	102.2	0.0752		100.0562	100.1	0.1443		103.0884	103.1	0.0000		99.5
Chloridazon-desphenyl	146.0 -...	0.0842		9.4229	94.2	19.4046	97.0	48.8804	97.8	99.5835	99.6	196.6906	98.3	501.5482	100.3	1020.7517	102.1	0.0473		118.7403	118.7	0.0000		123.3309	123.3	0.0000		48.0
Chloridazon-methyl-desphenyl	160.0 -...	0.0000		9.6489	96.5	19.1230	95.6	49.6773	99.4	101.7110	101.7	202.2343	101.1	507.7204	101.5	1013.4379	101.3	0.0860		100.4924	100.5	0.0154		104.0213	104.0	0.0000		77.6
Chlorpyrifos	349.9 -...	0.0000		6.3233	63.2	21.1044	105.5	44.2646	88.5	87.7354	87.7	230.4209	115.2	497.6379	99.5	1005.0455	100.5	1.1282		42.3430	42.3	0.0000		40.5051	40.5	0.0000		39.5
Chlortoluron (Chlorotoluron)	213.1 -...	0.0000		9.3136	93.1	18.6633	93.3	49.2509	98.5	101.8758	101.9	204.7478	102.4	495.9656	99.2	1012.0544	101.2	0.2146		99.2415	99.2	0.0000		105.8249	105.8	0.0000		79.3
Deisopropylatrazine	174.0 -...	0.0000		9.5353	95.4	19.6563	98.3	49.8150	99.6	103.1062	103.1	206.2434	103.1	518.7587	103.8	1014.7753	101.5	0.0467		105.1516	105.2	0.0374		104.3119	104.3	0.0167		103.5
Desethylatrazine	188.1 -...	0.0000		9.5455	95.5	19.1568	95.8	50.0757	100.2	104.0118	104.0	207.9635	104.0	510.5492	102.1	1003.2515	100.3	0.1191		107.3840	107.4	0.0622		112.0453	112.0	0.0000		52.2
Desethylterbutylazine	202.1 -...	0.0000		9.8941	98.9	19.6820	98.4	50.2870	100.6	103.0138	103.0	204.6884	102.3	512.9148	102.6	1010.6521	101.1	0.3222		105.3669	105.4	0.0000		112.3335	112.3	0.0000		52.6
Diuron	233.0 -...	0.0000		9.3922	93.9	19.1166	95.6	49.4369	98.9	102.5628	102.6	201.4063	100.7	509.5506	101.9	1008.2719	100.8	0.4077		101.7913	101.8	0.0000		108.0900	108.1	0.0000		81.1
Ethofumesate	304.1 -...	0.0000		9.4448	94.4	19.1199	95.6	45.2241	90.4	99.5664	99.6	203.1267	101.6	506.8196	101.4	1000.2152	100.0	0.4342		103.0517	103.1	0.0000		105.7015	105.7	0.0000		99.8
Isoproturon	207.1 -...	0.0000		9.7093	97.1	19.4901	97.5	49.0961	98.2	101.6062	101.6	204.3815	102.2	503.2161	100.6	1009.0831	100.9	0.2132		103.2964	103.3	0.0224		109.2091	109.2	0.0000		127.3
Lenacil	235.1 -...	0.0000		9.7504	97.5	19.6204	98.1	51.5417	103.1	105.7330	105.7	208.5570	104.3	520.7366	104.1	983.8666	98.4	0.1994		104.9982	105.0	0.0866		110.3429	110.3	0.0000		52.2
Metalaxyl	280.1 -...	0.0000		9.1744	91.7	19.0020	95.0	49.9733	99.9	102.5986	102.6	205.2550	102.6	497.9926	99.6	1012.8326	101.3	0.1247		99.9160	99.9	0.0298		104.3394	104.3	0.0000		47.7
Metamitron	203.1 -...	0.0000		9.1850	91.8	20.2199	101.1	50.7015	101.4	102.4198	102.4	200.4870	100.2	515.3685	103.1	1013.9303	101.4	0.0000		98.8182	98.8	0.0000		105.9201	105.9	0.0000		83.8
Metazachlor	278.1 -...	0.0000		9.6050	96.1	19.1691	95.8	49.7336	99.5	105.0914	105.1	207.4960	103.7	513.0757	102.6	1006.7559	100.7	0.3162		112.2599	112.3	0.0971		115.6858	115.7	0.0833		83.0
Metolachlor	284.1 -...	0.0000		9.4758	94.8	19.5262	97.6	49.5671	99.1	100.4946	100.5	203.1694	101.6	499.5331	99.9	1009.7702	101.0	0.2922		96.0150	96.0	0.1698		101.2075	101.2	0.0000		74.0

+ MRM (160.0 -> 87.9) Blank-1-r001.d

Type: Linear

Origin: Blank off...

Weight: None

Chloridazon-methyl-desphenyl - 7 Levels, 7 Levels Used, 14 Points, 13 Points Used, 9 QCs

y = 3155.411079 * x + 6774.820160

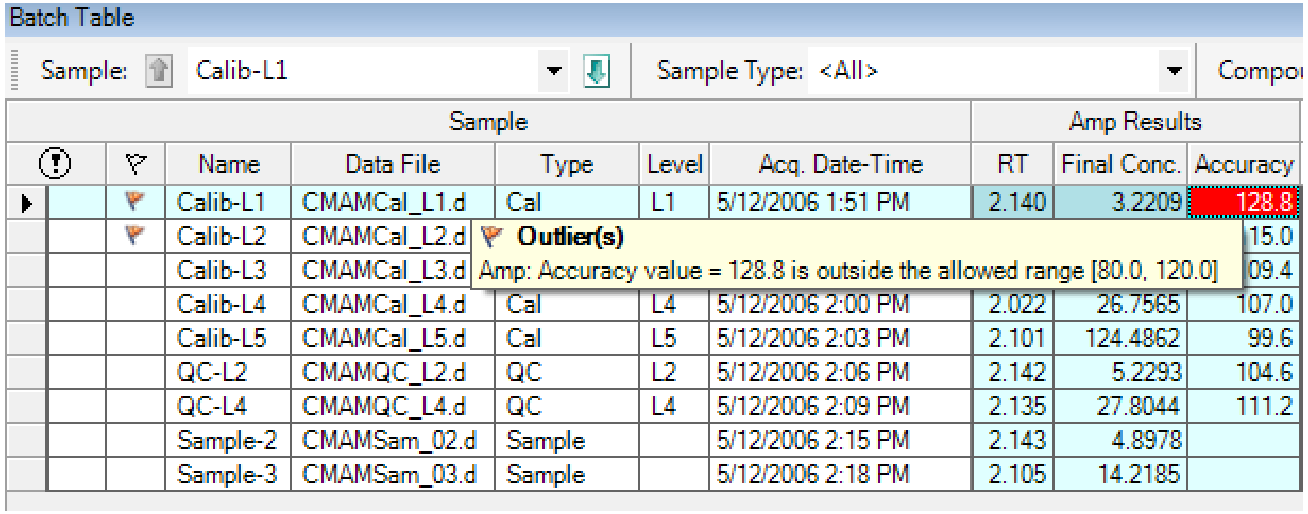
R^2 = 0.99872732

Type:Linear, Origin:Blank offset, Weight:None

Modified | TapWater_Blank | Chloridazon-methyl-desphenyl | 28 Compounds (28 total including ISTDs)

2 Configurable Views: both take advantage of Outliers

Batch-at-a-Glance


Batch Table

Sample: Calib-L1 Sample Type: <All> Compo

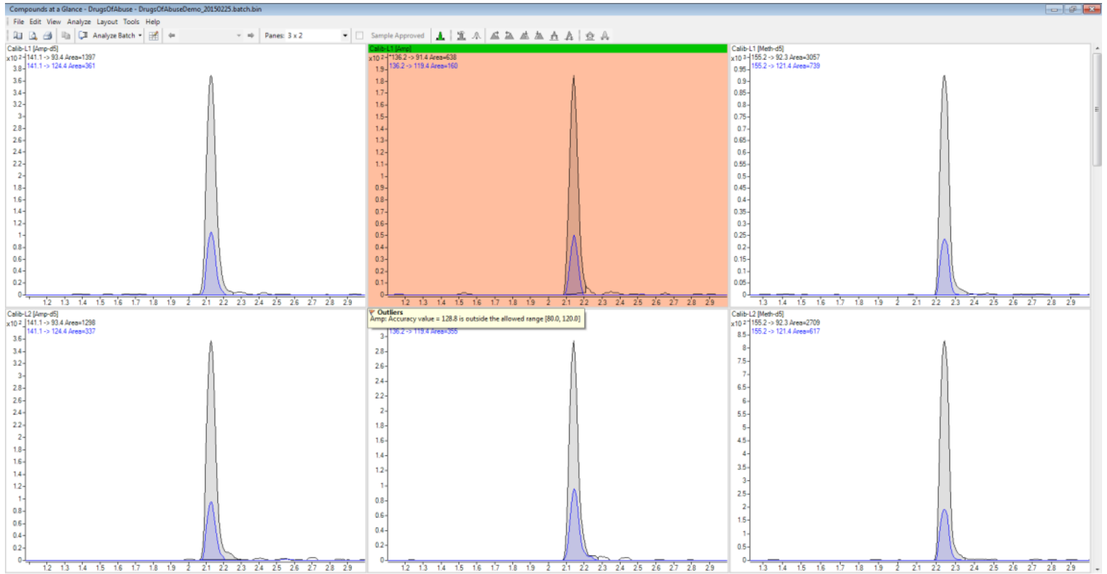
			Sample					Amp Results		
	(!)	🚩	Name	Data File	Type	Level	Acq. Date-Time	RT	Final Conc.	Accuracy
▶		🚩	Calib-L1	CMAMCal_L1.d	Cal	L1	5/12/2006 1:51 PM	2.140	3.2209	128.8
		🚩	Calib-L2	CMAMCal_L2.d						15.0
			Calib-L3	CMAMCal_L3.d						09.4
			Calib-L4	CMAMCal_L4.d	Cal	L4	5/12/2006 2:00 PM	2.022	26.7565	107.0
			Calib-L5	CMAMCal_L5.d	Cal	L5	5/12/2006 2:03 PM	2.101	124.4862	99.6
			QC-L2	CMAMQC_L2.d	QC	L2	5/12/2006 2:06 PM	2.142	5.2293	104.6
			QC-L4	CMAMQC_L4.d	QC	L4	5/12/2006 2:09 PM	2.135	27.8044	111.2
			Sample-2	CMAMSam_02.d	Sample		5/12/2006 2:15 PM	2.143	4.8978	
			Sample-3	CMAMSam_03.d	Sample		5/12/2006 2:18 PM	2.105	14.2185	

🚩 **Outlier(s)**

Amp: Accuracy value = 128.8 is outside the allowed range [80.0, 120.0]

http://www.chem.agilent.com/en-US/products-services/Software-Informatics/MassHunter-Workstation-Software/Pages/Batch_at_a_glance_demo.aspx

Compounds-at-a-Glance

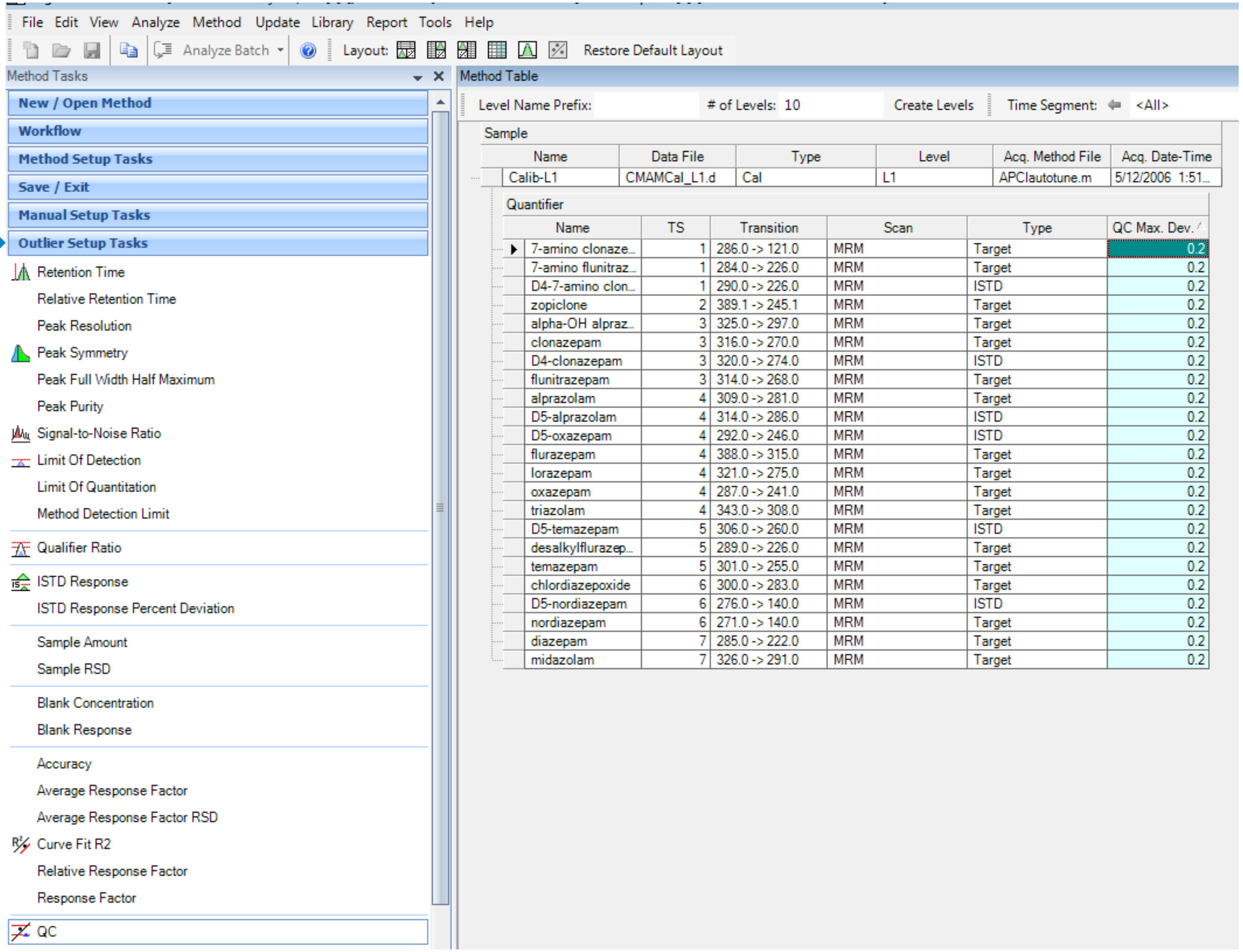


http://www.chem.agilent.com/en-US/products-services/Software-Informatics/MassHunter-Workstation-Software/Pages/quant_flat_table.aspx

Outlier Options: Configured in the Method

40+ Outliers can be configured (B.07.01):

1. Retention Time
2. Relative Retention Time
3. Peak Resolution
4. Peak Symmetry
5. Peak Purity
6. Signal-to-noise Ratio
7. Limit of Detection
8. Limit of Quantitation
9. Method Detection Limit
10. Qualifier Ratio
11. Internal Standard Response
12. Internal Standard % Deviation
13. Sample Amount
14. Sample % RSD
15. Blank Concentration
16. Blank Response
17. Accuracy
18. Average Response Factor
19. Average Response Factor %RSD
20. Curve Fit R^2
21. Relative Response Factor
22. Response Factor
23. QC Max Deviation
24. QC Relative Standard Deviation
25. QC LCS Recovery
26. CC Average Response Factor
27. CC Internal Std Response Ratio
28. CC Relative Response Factor
29. CC Response Ratio
30. CC Retention Time
31. Matrix Spike
32. Matrix Spike % Difference
33. Matrix Spike Percent Recovery
34. Matrix Spike Group Recovery
35. Surrogate
36. Surrogate % Recovery
37. Response Check
38. Mass accuracy
39. Mass Match Score
40. Library Match Score
41. ***Custom Calculation***



Level Name Prefix:

# of Levels: 10

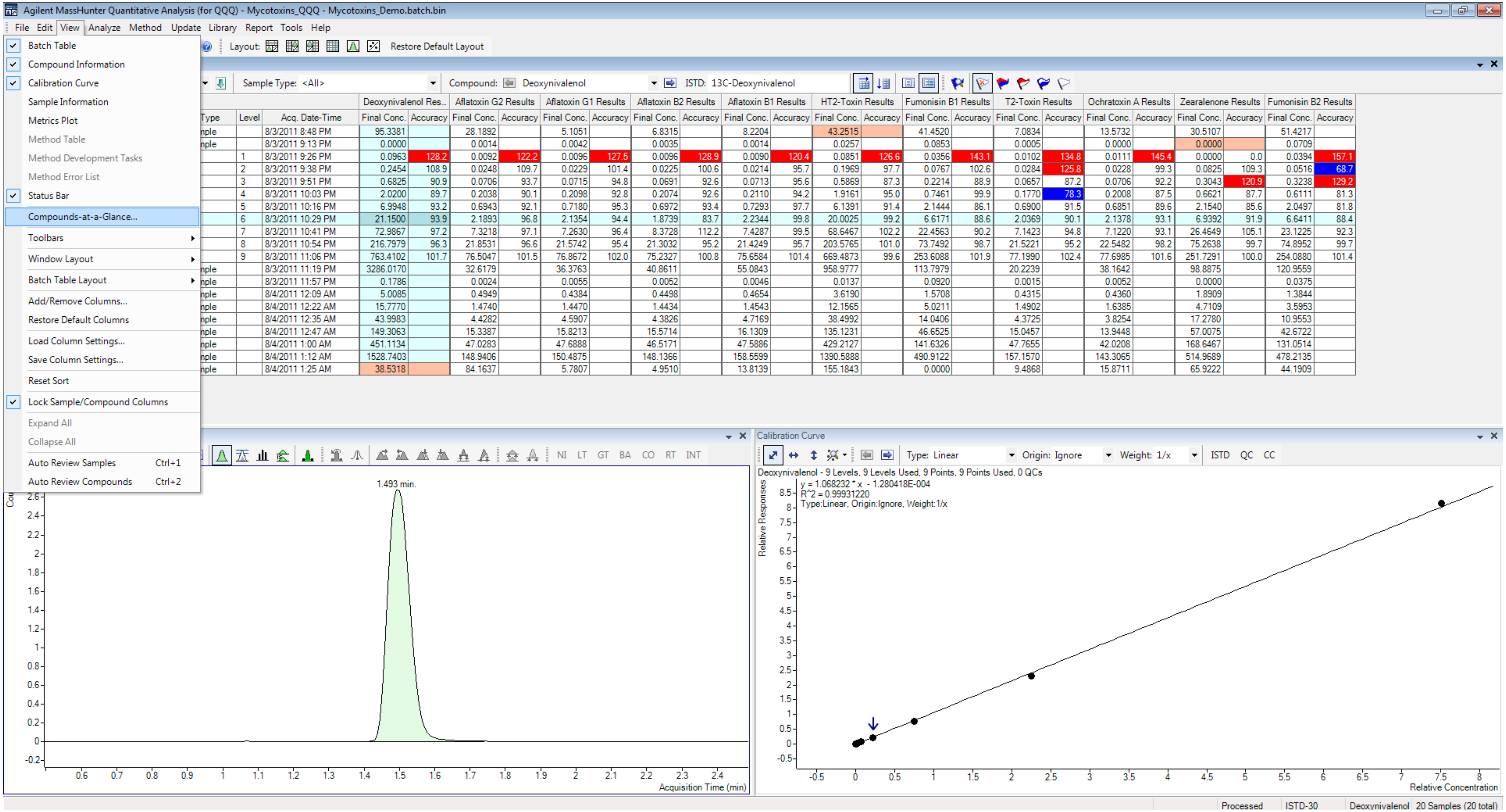
Time Segment: <All>

Sample

Name	Data File	Type	Level	Acq. Method File	Acq. Date-Time
Calib-L1	CMAMCal_L1.d	Cal	L1	APClautotune.m	5/12/2006 1:51...

Quantifier

Name	TS	Transition	Scan	Type	QC Max. Dev.
7-amino clonaze...	1	286.0 -> 121.0	MRM	Target	0.2
7-amino flunitraz...	1	284.0 -> 226.0	MRM	Target	0.2
D4-7-amino clon...	1	290.0 -> 226.0	MRM	ISTD	0.2
zopiclone	2	389.1 -> 245.1	MRM	Target	0.2
alpha-OH alpraz...	3	325.0 -> 297.0	MRM	Target	0.2
clonazepam	3	316.0 -> 270.0	MRM	Target	0.2
D4-clonazepam	3	320.0 -> 274.0	MRM	ISTD	0.2
flunitrazepam	3	314.0 -> 268.0	MRM	Target	0.2
alprazolam	4	309.0 -> 281.0	MRM	Target	0.2
D5-alprazolam	4	314.0 -> 286.0	MRM	ISTD	0.2
D5-oxazepam	4	292.0 -> 246.0	MRM	ISTD	0.2
flurazepam	4	388.0 -> 315.0	MRM	Target	0.2
lorazepam	4	321.0 -> 275.0	MRM	Target	0.2
oxazepam	4	287.0 -> 241.0	MRM	Target	0.2
triazolam	4	343.0 -> 308.0	MRM	Target	0.2
D5-temazepam	5	306.0 -> 260.0	MRM	ISTD	0.2
desalkylflurazep...	5	289.0 -> 226.0	MRM	Target	0.2
temazepam	5	301.0 -> 255.0	MRM	Target	0.2
chlordiazepoxide	6	300.0 -> 283.0	MRM	Target	0.2
D5-nordiazepam	6	276.0 -> 140.0	MRM	ISTD	0.2
nordiazepam	6	271.0 -> 140.0	MRM	Target	0.2
diazepam	7	285.0 -> 222.0	MRM	Target	0.2
midazolam	7	326.0 -> 291.0	MRM	Target	0.2



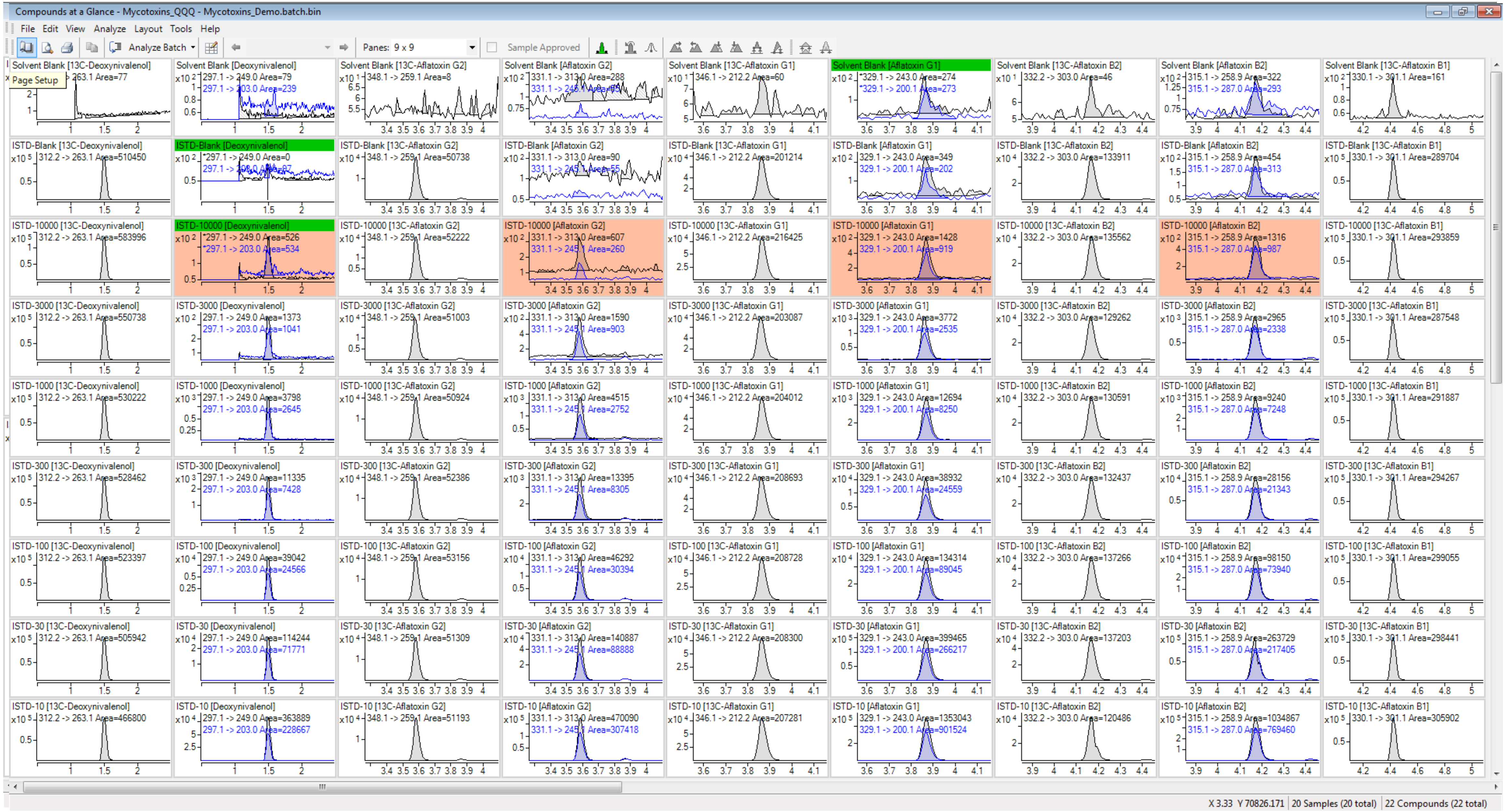
Sample Type: <All>
Compound: Deoxynivalenol
ISTD: 13C-Deoxynivalenol

			Deoxynivalenol Res...		Aflatoxin G2 Results		Aflatoxin G1 Results		Aflatoxin B2 Results		Aflatoxin B1 Results	
Type	Level	Acq. Date-Time	Final Conc.	Accuracy	Final Conc.	Accuracy	Final Conc.	Accuracy	Final Conc.	Accuracy	Final Conc.	Accuracy
nple		8/3/2011 8:48 PM	95.3381		28.1892		5.1051		6.8315		8.2204	
nple		8/3/2011 9:13 PM	0.0000		0.0014		0.0042		0.0035		0.0014	
	1	8/3/2011 9:26 PM	0.0963	128.2	0.0092	122.2	0.0096	127.5	0.0096	128.9	0.0090	120.4
	2	8/3/2011 9:38 PM	0.2454	108.9	0.0248	109.7	0.0229	101.4	0.0225	100.6	0.0214	95.7
	3	8/3/2011 9:51 PM	0.6825	90.9	0.0706	93.7	0.0715	94.8	0.0691	92.6	0.0713	95.6
	4	8/3/2011 10:03 PM	2.0200	89.7	0.2038	90.1	0.2098	92.8	0.2074	92.6	0.2110	94.2
	5	8/3/2011 10:16 PM	6.9948	93.2	0.6943	92.1	0.7180	95.3	0.6972	93.4	0.7293	97.7
	6	8/3/2011 10:29 PM	21.1500	93.9	2.1893	96.8	2.1354	94.4	1.8739	83.7	2.2344	99.8
	7	8/3/2011 10:41 PM	72.9867	97.2	7.3218	97.1	7.2630	96.4	8.3728	112.2	7.4287	99.5
	8	8/3/2011 10:54 PM	216.7979	96.3	21.8531	96.6	21.5742	95.4	21.3032	95.2	21.4249	95.7
	9	8/3/2011 11:06 PM	763.4102	101.7	76.5047	101.5	76.8672	102.0	75.2327	100.8	75.6584	101.4
nple		8/3/2011 11:19 PM	3286.0170		32.6179		36.3763		40.8611		55.0843	
nple		8/3/2011 11:57 PM	0.1786		0.0024		0.0055		0.0052		0.0046	
nple		8/4/2011 12:09 AM	5.0085		0.4949		0.4384		0.4498		0.4654	
nple		8/4/2011 12:22 AM	15.7770		1.4740		1.4470		1.4434		1.4543	
nple		8/4/2011 12:35 AM	43.9983		4.4282		4.5907		4.3826		4.7169	
nple		8/4/2011 12:47 AM	149.3063		15.3387		15.8213		15.5714		16.1309	
nple		8/4/2011 1:00 AM	451.1134		47.0283		47.6888		46.5171		47.5886	
nple		8/4/2011 1:12 AM	1528.7403		148.9406		150.4875		148.1366		158.5599	
nple		8/4/2011 1:25 AM	38.5318		84.1637		5.7807		4.9510		13.8139	

		HT2-Toxin Results		Fumonisin B1 Results		T2-Toxin Results		Ochratoxin A Results		Zearalenone Results		Fumonisin B2 Results	
Level	Acq. Date-Time	Final Conc.	Accuracy	Final Conc.	Accuracy	Final Conc.	Accuracy	Final Conc.	Accuracy	Final Conc.	Accuracy	Final Conc.	Accuracy
	8/3/2011 8:48 PM	43.2515		41.4520		7.0834		13.5732		30.5107		51.4217	
	8/3/2011 9:13 PM	0.0257		0.0853		0.0005		0.0000		0.0000		0.0709	
1	8/3/2011 9:26 PM	0.0851	126.6	0.0356	143.1	0.0102	134.8	0.0111	145.4	0.0000	0.0	0.0394	157.1
2	8/3/2011 9:38 PM	0.1969	97.7	0.0767	102.6	0.0284	125.8	0.0228	99.3	0.0825	109.3	0.0516	68.7
3	8/3/2011 9:51 PM	0.5869	87.3	0.2214	88.9	0.0657	87.2	0.0706	92.2	0.3043	120.9	0.3238	129.2
4	8/3/2011 10:03 PM	1.9161	95.0	0.7461	99.9	0.1770	78.3	0.2008	87.5	0.6621	87.7	0.6111	81.3
5	8/3/2011 10:16 PM	6.1391	91.4	2.1444	86.1	0.6900	91.5	0.6851	89.6	2.1540	85.6	2.0497	81.8
6	8/3/2011 10:29 PM	20.0025	99.2	6.6171	88.6	2.0369	90.1	2.1378	93.1	6.9392	91.9	6.6411	88.4
7	8/3/2011 10:41 PM	68.6467	102.2	22.4563	90.2	7.1423	94.8	7.1220	93.1	26.4649	105.1	23.1225	92.3
8	8/3/2011 10:54 PM	203.5765	101.0	73.7492	98.7	21.5221	95.2	22.5482	98.2	75.2638	99.7	74.8952	99.7
9	8/3/2011 11:06 PM	669.4873	99.6	253.6088	101.9	77.1990	102.4	77.6985	101.6	251.7291	100.0	254.0880	101.4
	8/3/2011 11:19 PM	958.9777		113.7979		20.2239		38.1642		98.8875		120.9559	
	8/3/2011 11:57 PM	0.0137		0.0920		0.0015		0.0052		0.0000		0.0375	
	8/4/2011 12:09 AM	3.6190		1.5708		0.4315		0.4360		1.8909		1.3844	
	8/4/2011 12:22 AM	12.1565		5.0211		1.4902		1.6385		4.7109		3.5953	
	8/4/2011 12:35 AM	38.4992		14.0406		4.3725		3.8254		17.2780		10.9553	
	8/4/2011 12:47 AM	135.1231		46.6525		15.0457		13.9448		57.0075		42.6722	
	8/4/2011 1:00 AM	429.2127		141.6326		47.7655		42.0208		168.6467		131.0514	
	8/4/2011 1:12 AM	1390.5888		490.9122		157.1570		143.3065		514.9689		478.2135	
	8/4/2011 1:25 AM	155.1843		0.0000		9.4868		15.8711		65.9222		44.1909	

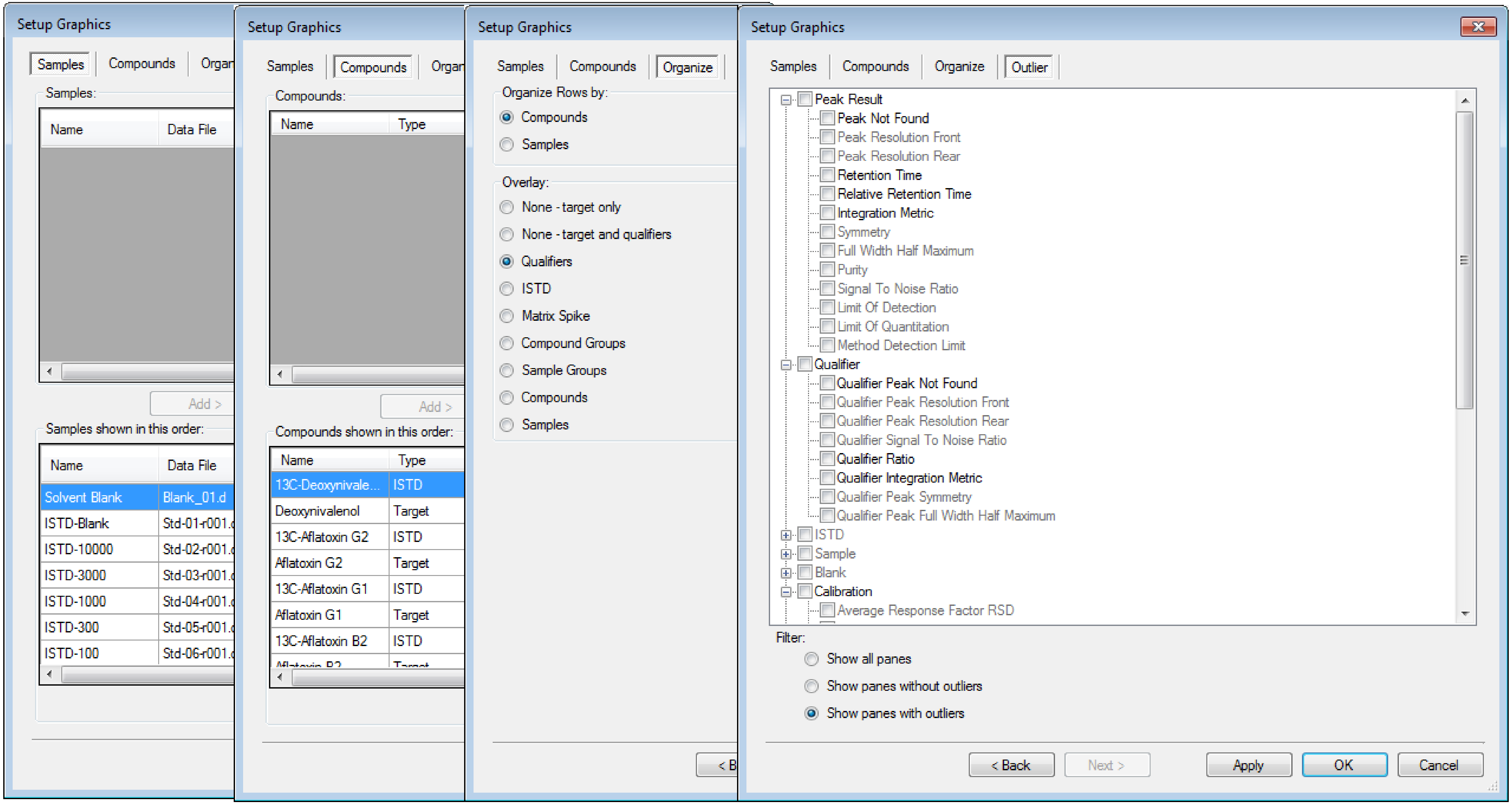
Type: Linear
Origin: Ignore
Weight: 1/x

Deoxynivalenol - 9 Levels, 9 Levels Used, 9 Points, 9 Points Used, 0 QCs
y = 1.068232 * x - 1.280418E-004
R^2 = 0.99931220
Type:Linear, Origin:Ignore, Weight:1/x



	[13C-Deoxynivalenol]	[Deoxynivalenol]	[13C-Aflatoxin G2]	[Aflatoxin G2]	[13C-Aflatoxin G1]	[Aflatoxin G1]	[13C-Aflatoxin B2]	[Aflatoxin B2]	[13C-Aflatoxin B1]
Solvent Blank	263.1 Area=77	297.1 -> 249.0 Area=79 297.1 -> 203.0 Area=239	348.1 -> 259.1 Area=8	331.1 -> 313.0 Area=288 331.1 -> 245.1 Area=[illegible]	346.1 -> 212.2 Area=60	*329.1 -> 243.0 Area=274 *329.1 -> 200.1 Area=273	332.2 -> 303.0 Area=46	315.1 -> 258.9 Area=322 315.1 -> 287.0 Area=293	330.1 -> 301.1 Area=161
ISTD-Blank	312.2 -> 263.1 Area=510450	*297.1 -> 249.0 Area=0 297.1 -> 203.0 Area=87	348.1 -> 259.1 Area=50738	331.1 -> 313.0 Area=90 331.1 -> 245.1 Area=55	346.1 -> 212.2 Area=201214	329.1 -> 243.0 Area=349 329.1 -> 200.1 Area=202	332.2 -> 303.0 Area=133911	315.1 -> 258.9 Area=454 315.1 -> 287.0 Area=313	330.1 -> 301.1 Area=289704
ISTD-10000	312.2 -> 263.1 Area=583996	*297.1 -> 249.0 Area=526 *297.1 -> 203.0 Area=534	348.1 -> 259.1 Area=52222	331.1 -> 313.0 Area=607 331.1 -> 245.1 Area=260	346.1 -> 212.2 Area=216425	329.1 -> 243.0 Area=1428 329.1 -> 200.1 Area=919	332.2 -> 303.0 Area=135562	315.1 -> 258.9 Area=1316 315.1 -> 287.0 Area=987	330.1 -> 301.1 Area=293859
ISTD-3000	312.2 -> 263.1 Area=550738	297.1 -> 249.0 Area=1373 297.1 -> 203.0 Area=1041	348.1 -> 259.1 Area=51003	331.1 -> 313.0 Area=1590 331.1 -> 245.1 Area=903	346.1 -> 212.2 Area=203087	329.1 -> 243.0 Area=3772 329.1 -> 200.1 Area=2535	332.2 -> 303.0 Area=129262	315.1 -> 258.9 Area=2965 315.1 -> 287.0 Area=2338	330.1 -> 301.1 Area=287548
ISTD-1000	312.2 -> 263.1 Area=530222	297.1 -> 249.0 Area=3798 297.1 -> 203.0 Area=2645	348.1 -> 259.1 Area=50924	331.1 -> 313.0 Area=4515 331.1 -> 245.1 Area=2752	346.1 -> 212.2 Area=204012	329.1 -> 243.0 Area=12694 329.1 -> 200.1 Area=8250	332.2 -> 303.0 Area=130591	315.1 -> 258.9 Area=9240 315.1 -> 287.0 Area=7248	330.1 -> 301.1 Area=291887
ISTD-300	312.2 -> 263.1 Area=528462	297.1 -> 249.0 Area=11335 297.1 -> 203.0 Area=7428	348.1 -> 259.1 Area=52386	331.1 -> 313.0 Area=13395 331.1 -> 245.1 Area=8305	346.1 -> 212.2 Area=208693	329.1 -> 243.0 Area=38932 329.1 -> 200.1 Area=24559	332.2 -> 303.0 Area=132437	315.1 -> 258.9 Area=28156 315.1 -> 287.0 Area=21343	330.1 -> 301.1 Area=294267
ISTD-100	312.2 -> 263.1 Area=523397	297.1 -> 249.0 Area=39042 297.1 -> 203.0 Area=24566	348.1 -> 259.1 Area=53156	331.1 -> 313.0 Area=46292 331.1 -> 245.1 Area=30394	346.1 -> 212.2 Area=208728	329.1 -> 243.0 Area=134314 329.1 -> 200.1 Area=89045	332.2 -> 303.0 Area=137266	315.1 -> 258.9 Area=98150 315.1 -> 287.0 Area=73940	330.1 -> 301.1 Area=299055
ISTD-30	312.2 -> 263.1 Area=505942	297.1 -> 249.0 Area=114244 297.1 -> 203.0 Area=71771	348.1 -> 259.1 Area=51309	331.1 -> 313.0 Area=140887 331.1 -> 245.1 Area=88888	346.1 -> 212.2 Area=208300	329.1 -> 243.0 Area=399465 329.1 -> 200.1 Area=266217	332.2 -> 303.0 Area=137203	315.1 -> 258.9 Area=263729 315.1 -> 287.0 Area=217405	330.1 -> 301.1 Area=298441
ISTD-10	312.2 -> 263.1 Area=466800	297.1 -> 249.0 Area=363889 297.1 -> 203.0 Area=228667	348.1 -> 259.1 Area=51193	331.1 -> 313.0 Area=470090 331.1 -> 245.1 Area=307418	346.1 -> 212.2 Area=207281	329.1 -> 243.0 Area=1353043 329.1 -> 200.1 Area=901524	332.2 -> 303.0 Area=120486	315.1 -> 258.9 Area=1034867 315.1 -> 287.0 Area=769460	330.1 -> 301.1 Area=305902

X 3.33 Y 70826.171 | 20 Samples (20 total) | 22 Compounds (22 total)



Samples:

Name	Data File

Samples shown in this order:

Name	Data File
Solvent Blank	Blank_01.d
ISTD-Blank	Std-01-r001.
ISTD-10000	Std-02-r001.
ISTD-3000	Std-03-r001.
ISTD-1000	Std-04-r001.
ISTD-300	Std-05-r001.
ISTD-100	Std-06-r001.

Compounds:

Name	Type

Compounds shown in this order:

Name	Type
13C-Deoxynivale...	ISTD
Deoxynivalenol	Target
13C-Aflatoxin G2	ISTD
Aflatoxin G2	Target
13C-Aflatoxin G1	ISTD
Aflatoxin G1	Target
13C-Aflatoxin B2	ISTD

Organize Rows by:

● Compounds
○ Samples

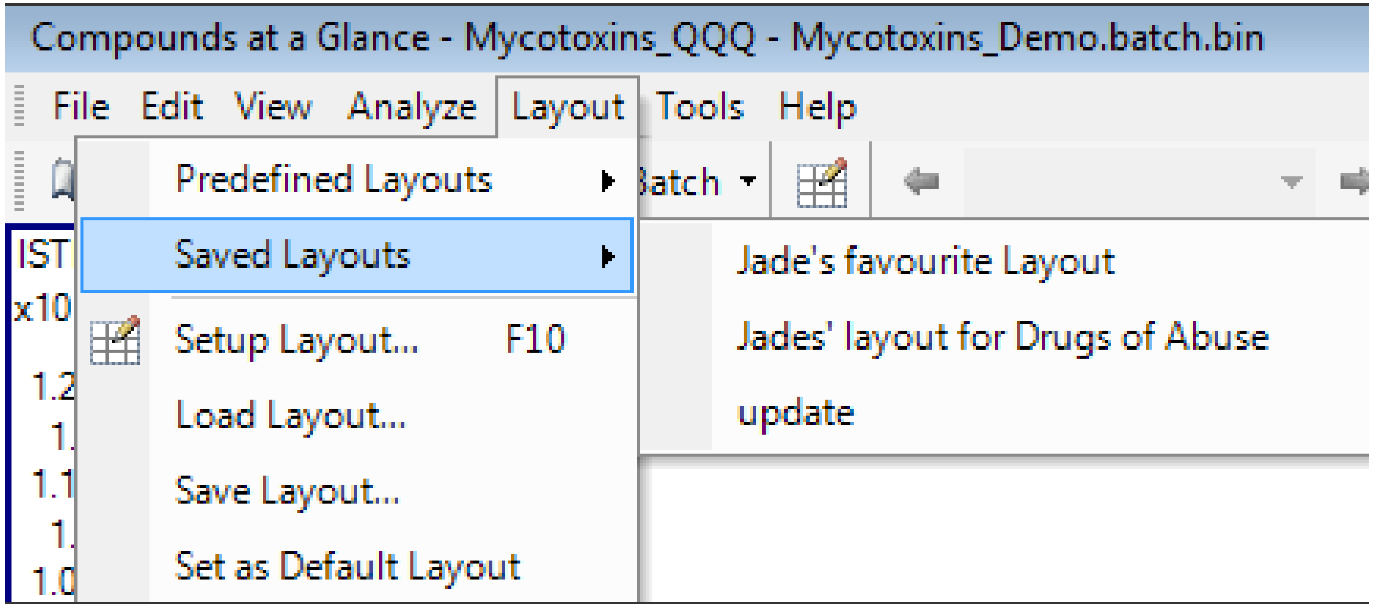
Overlay:

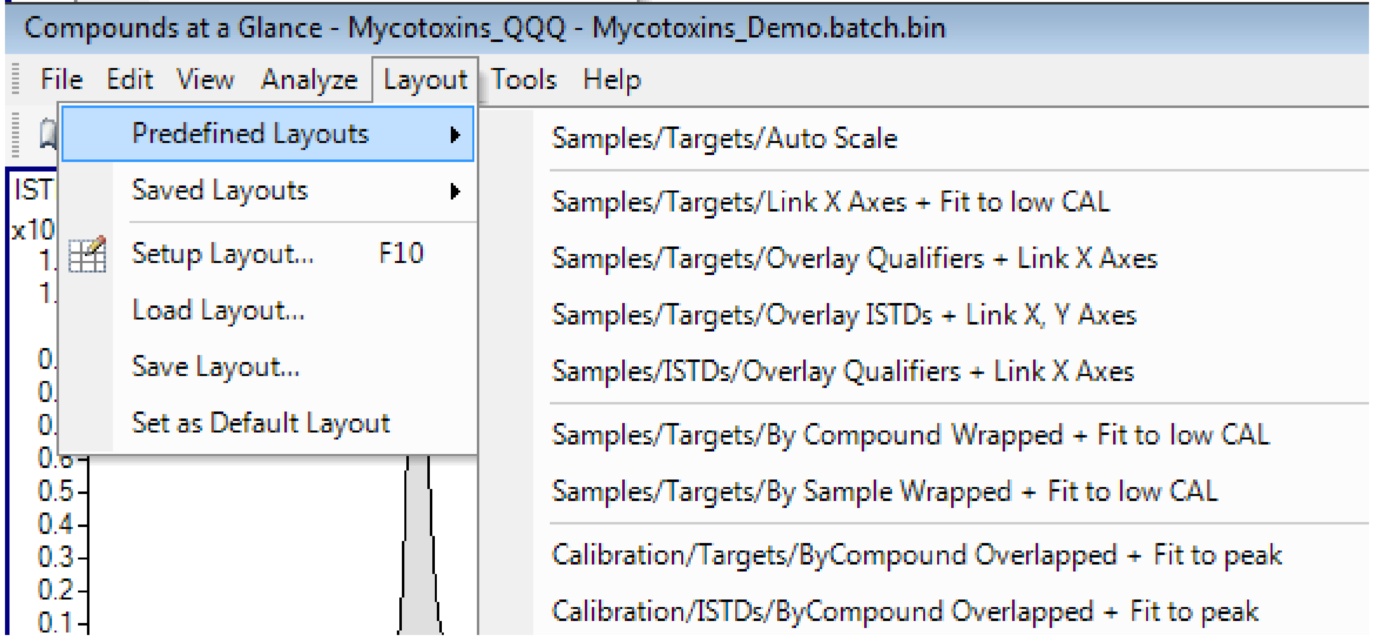
○ None - target only
○ None - target and qualifiers
● Qualifiers
○ ISTD
○ Matrix Spike
○ Compound Groups
○ Sample Groups
○ Compounds
○ Samples

- ☐ Peak Result
  - ☐ Peak Not Found
  - ☐ Peak Resolution Front
  - ☐ Peak Resolution Rear
  - ☐ Retention Time
  - ☐ Relative Retention Time
  - ☐ Integration Metric
  - ☐ Symmetry
  - ☐ Full Width Half Maximum
  - ☐ Purity
  - ☐ Signal To Noise Ratio
  - ☐ Limit Of Detection
  - ☐ Limit Of Quantitation
  - ☐ Method Detection Limit
- ☐ Qualifier
  - ☐ Qualifier Peak Not Found
  - ☐ Qualifier Peak Resolution Front
  - ☐ Qualifier Peak Resolution Rear
  - ☐ Qualifier Signal To Noise Ratio
  - ☐ Qualifier Ratio
  - ☐ Qualifier Integration Metric
  - ☐ Qualifier Peak Symmetry
  - ☐ Qualifier Peak Full Width Half Maximum
- ☐ ISTD
- ☐ Sample
- ☐ Blank
- ☐ Calibration
  - ☐ Average Response Factor RSD

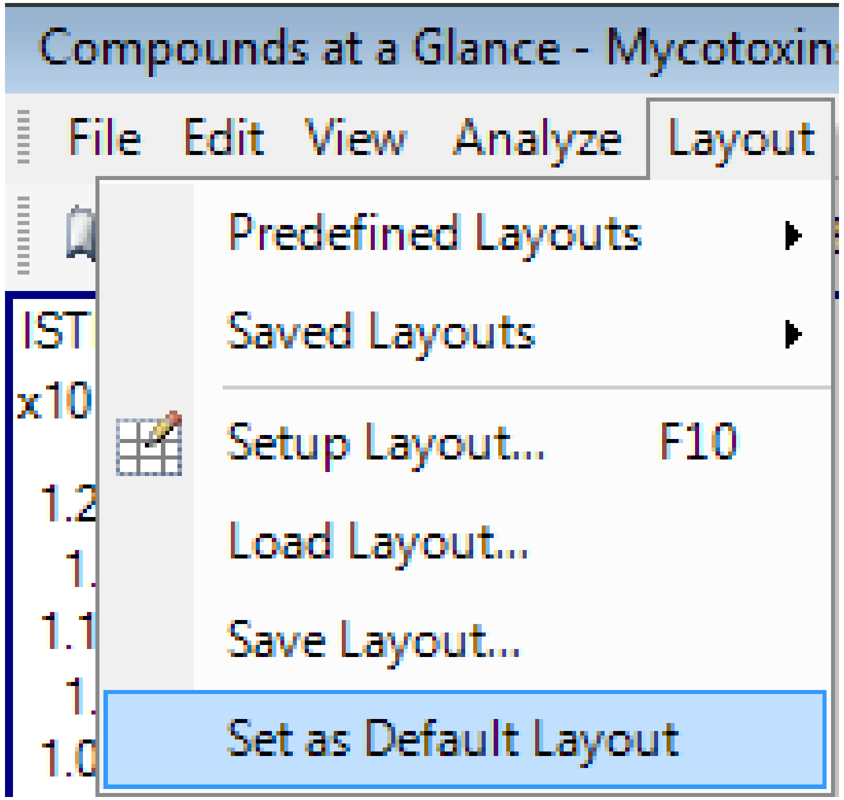
Filter:

○ Show all panes
○ Show panes without outliers
● Show panes with outliers


Compounds at a Glance - Mycotoxins_QQQ - Mycotoxins_Demo.batch.bin
File
Edit
View
Analyze
Layout
Tools
Help
Predefined Layouts
Saved Layouts
Setup Layout... F10
Load Layout...
Save Layout...
Set as Default Layout
Batch
Jade's favourite Layout
Jades' layout for Drugs of Abuse
update
IST
x10
1.2
1.1
1.0


Compounds at a Glance - Mycotoxins_QQQ - Mycotoxins_Demo.batch.bin
File
Edit
View
Analyze
Layout
Tools
Help
Predefined Layouts
Saved Layouts
Setup Layout... F10
Load Layout...
Save Layout...
Set as Default Layout
Samples/Targets/Auto Scale
Samples/Targets/Link X Axes + Fit to low CAL
Samples/Targets/Overlay Qualifiers + Link X Axes
Samples/Targets/Overlay ISTDs + Link X, Y Axes
Samples/ISTDs/Overlay Qualifiers + Link X Axes
Samples/Targets/By Compound Wrapped + Fit to low CAL
Samples/Targets/By Sample Wrapped + Fit to low CAL
Calibration/Targets/ByCompound Overlapped + Fit to peak
Calibration/ISTDs/ByCompound Overlapped + Fit to peak
IST
x10
0.5
0.4
0.3
0.2
0.1

NEW in B.07.01

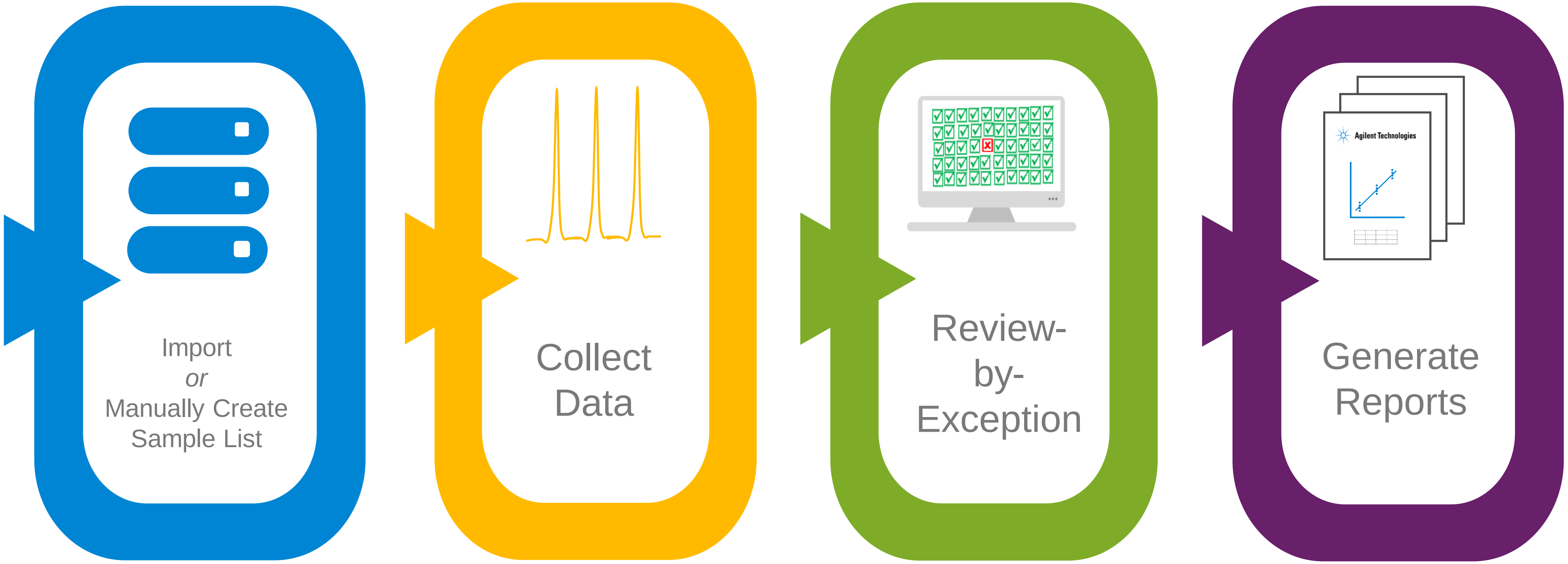

Compounds at a Glance - Mycotoxin
File
Edit
View
Analyze
Layout
Predefined Layouts
Saved Layouts
Setup Layout... F10
Load Layout...
Save Layout...
Set as Default Layout
IST
x10
1.2
1.1
1.0

Compounds at a Glance - Mycotoxins_QQQ - Mycotoxins_Demo.batch.bin

Outliers
Deoxynivalenol: Accuracy value = 128.2 is outside the allowed range [80.0, 120.0]

X 2.22 Y 146.775 | 20 Samples (20 total) | 22 Compounds (22 total)

MassHunter Quantative Analysis Workflow



Import
or
Manually Create
Sample List

Collect
Data

Review-
by-
Exception

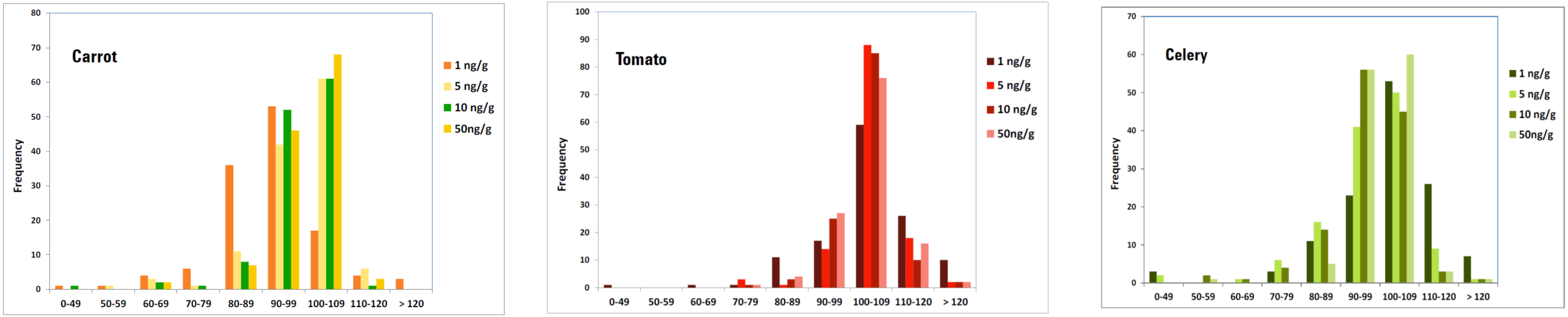
Generate
Reports

Excel Reports: A Case Study

Reduced Cost for Pesticides Residues Analysis by GC/MS/MS Using Mini-QuEChERS and a High Efficiency Source

Melissa Churley[1] and Joan Stevens[2] [1]Agilent Technologies Inc., 5301 Stevens Creek Blvd., Santa Clara, CA 95051 USA [2]Agilent Technologies Inc., 2850 Centerville Road, Wilmington, DE 19808 USA

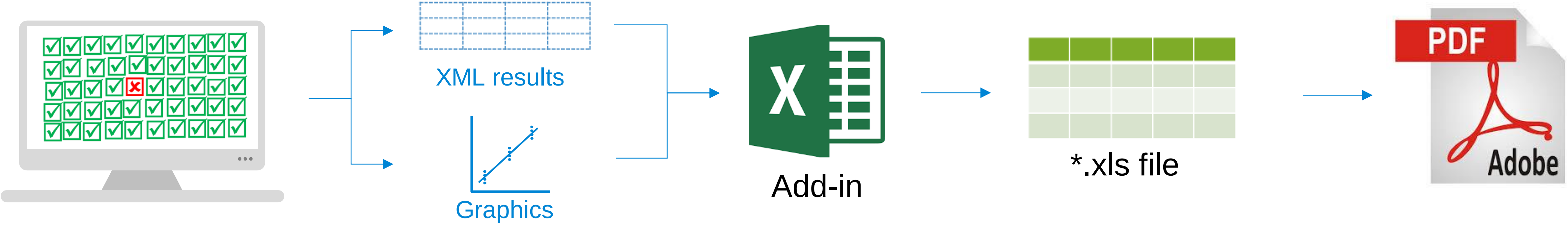
Distribution of Average Recoveries (n=6) for 126 Pesticides Spiked at 1, 5, 10 and 50 ng/g in Carrot, Tomato and Celery



These graphs took just **3 minutes** to prepare!

http://www.chem.agilent.com/Library/applications/5991-6069EN.pdf

How reports work in MassHunter Quantitative Analysis

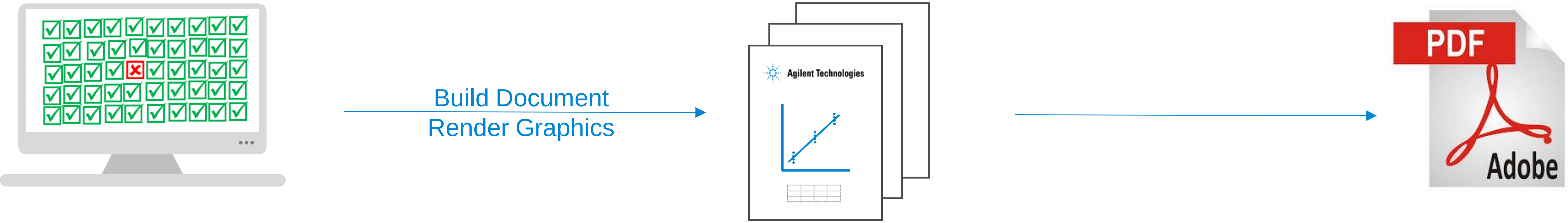


XML results

Graphics

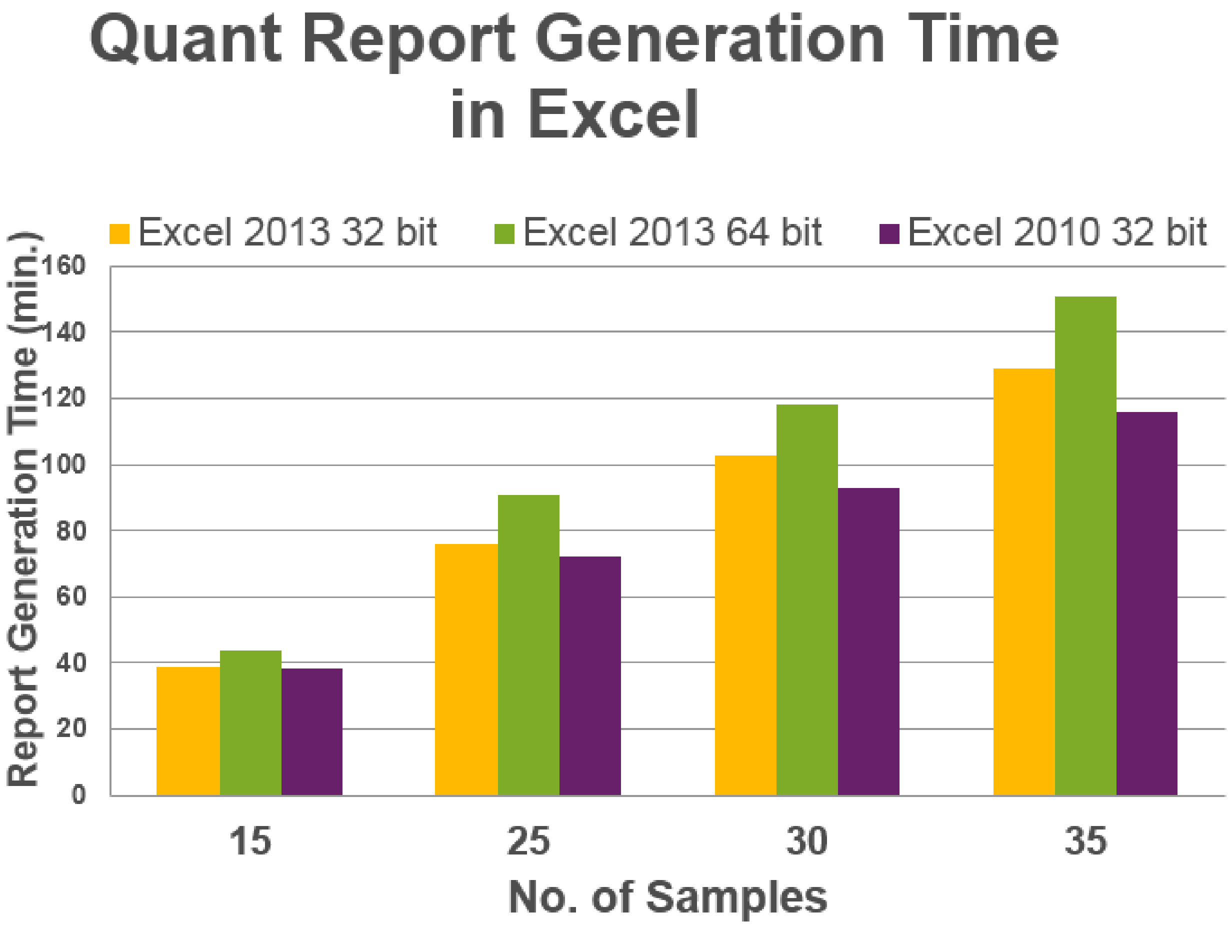
Add-in

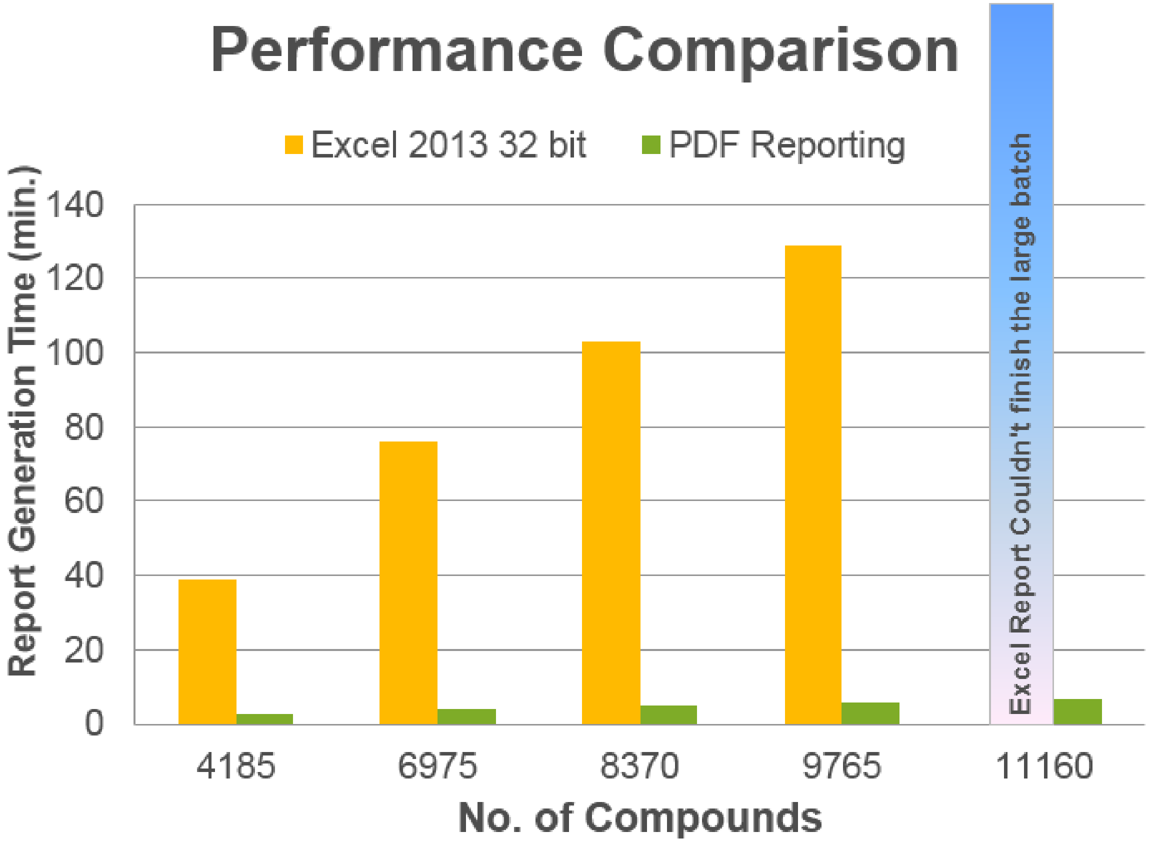
*.xls file



Build Document
Render Graphics

Significant Gains in Performance



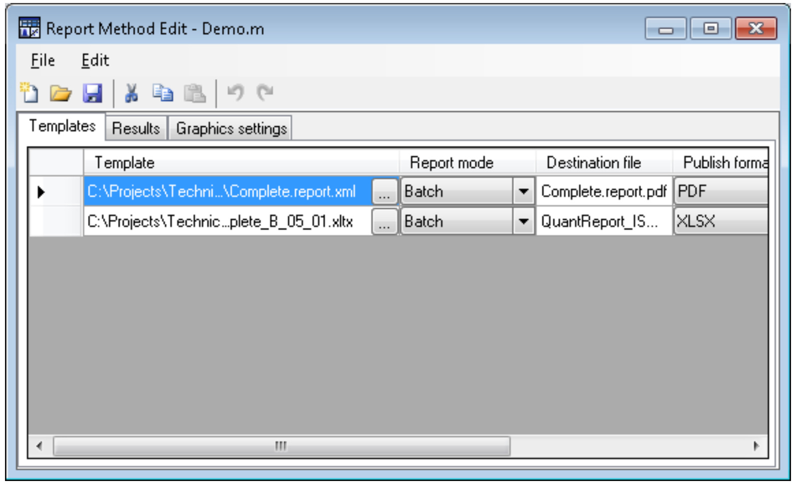


**Also benefit of modernization of code base

Automatically Generating Reports

Report Method

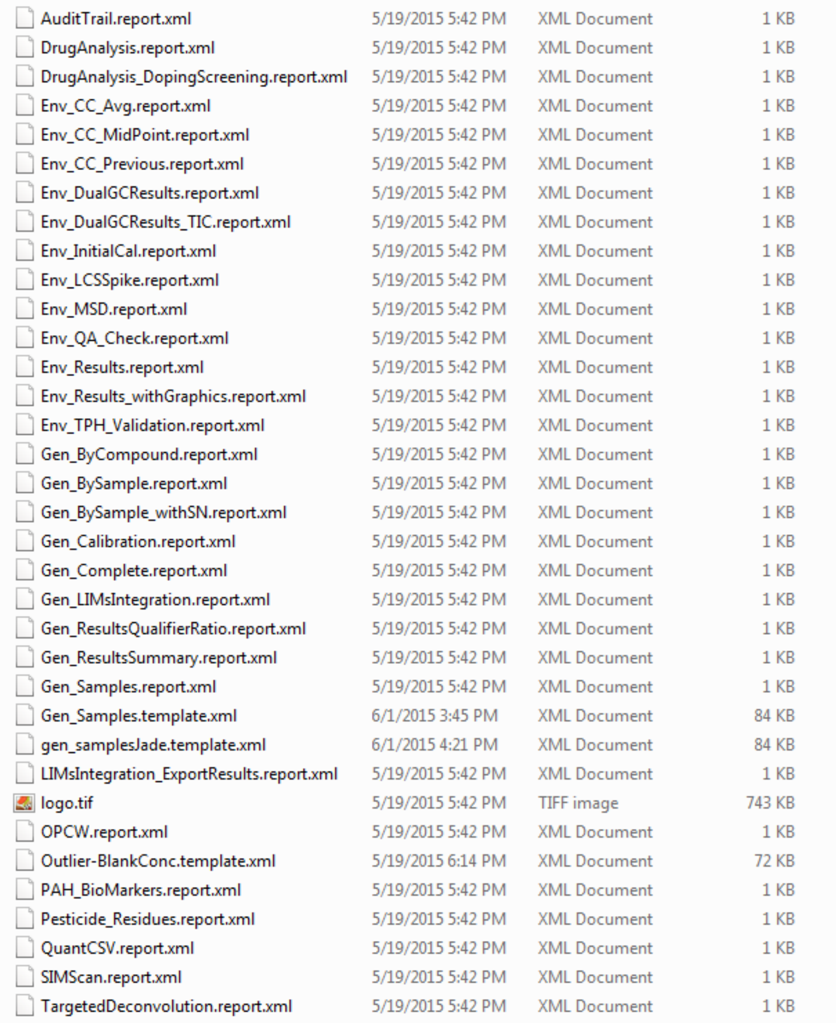
- Consolidates report settings
  - Templates, Graphic settings, post process
- Supports both Excel and PDF



	Template	Report mode	Destination file	Publish forma
▶	C:\Projects\Techni...\Complete.report.xml	Batch	Complete.report.pdf	PDF
	C:\Projects\Technic...plete_B_05_01.xltx	Batch	QuantReport_IS...	XLSX

Include Report Method in Unified Method

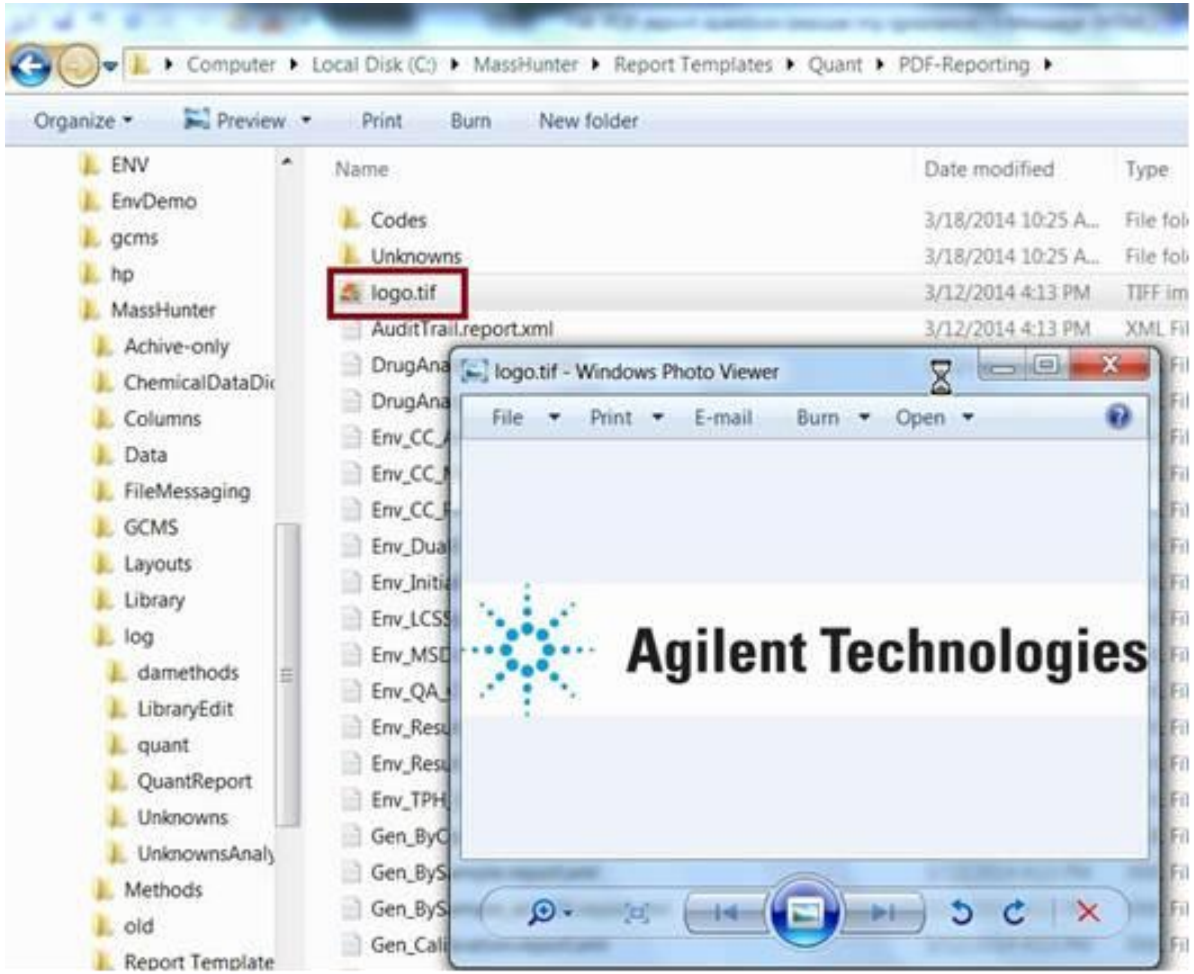
Dozens of PDF Report Templates Available at Installation



AuditTrail.report.xml	5/19/2015 5:42 PM	XML Document	1 KB
DrugAnalysis.report.xml	5/19/2015 5:42 PM	XML Document	1 KB
DrugAnalysis_DopingScreening.report.xml	5/19/2015 5:42 PM	XML Document	1 KB
Env_CC_Avg.report.xml	5/19/2015 5:42 PM	XML Document	1 KB
Env_CC_MidPoint.report.xml	5/19/2015 5:42 PM	XML Document	1 KB
Env_CC_Previous.report.xml	5/19/2015 5:42 PM	XML Document	1 KB
Env_DualGCResults.report.xml	5/19/2015 5:42 PM	XML Document	1 KB
Env_DualGCResults_TIC.report.xml	5/19/2015 5:42 PM	XML Document	1 KB
Env_InitialCal.report.xml	5/19/2015 5:42 PM	XML Document	1 KB
Env_LCSSpike.report.xml	5/19/2015 5:42 PM	XML Document	1 KB
Env_MSD.report.xml	5/19/2015 5:42 PM	XML Document	1 KB
Env_QA_Check.report.xml	5/19/2015 5:42 PM	XML Document	1 KB
Env_Results.report.xml	5/19/2015 5:42 PM	XML Document	1 KB
Env_Results_withGraphics.report.xml	5/19/2015 5:42 PM	XML Document	1 KB
Env_TPH_Validation.report.xml	5/19/2015 5:42 PM	XML Document	1 KB
Gen_ByCompound.report.xml	5/19/2015 5:42 PM	XML Document	1 KB
Gen_BySample.report.xml	5/19/2015 5:42 PM	XML Document	1 KB
Gen_BySample_withSN.report.xml	5/19/2015 5:42 PM	XML Document	1 KB
Gen_Calibration.report.xml	5/19/2015 5:42 PM	XML Document	1 KB
Gen_Complete.report.xml	5/19/2015 5:42 PM	XML Document	1 KB
Gen_LIMsIntegration.report.xml	5/19/2015 5:42 PM	XML Document	1 KB
Gen_ResultsQualifierRatio.report.xml	5/19/2015 5:42 PM	XML Document	1 KB
Gen_ResultsSummary.report.xml	5/19/2015 5:42 PM	XML Document	1 KB
Gen_Samples.report.xml	5/19/2015 5:42 PM	XML Document	1 KB
Gen_Samples.template.xml	6/1/2015 3:45 PM	XML Document	84 KB
gen_samplesJade.template.xml	6/1/2015 4:21 PM	XML Document	84 KB
LIMsIntegration_ExportResults.report.xml	5/19/2015 5:42 PM	XML Document	1 KB
logo.tif	5/19/2015 5:42 PM	TIFF image	743 KB
OPCW.report.xml	5/19/2015 5:42 PM	XML Document	1 KB
Outlier-BlankConc.template.xml	5/19/2015 6:14 PM	XML Document	72 KB
PAH_BioMarkers.report.xml	5/19/2015 5:42 PM	XML Document	1 KB
Pesticide_Residues.report.xml	5/19/2015 5:42 PM	XML Document	1 KB
QuantCSV.report.xml	5/19/2015 5:42 PM	XML Document	1 KB
SIMScan.report.xml	5/19/2015 5:42 PM	XML Document	1 KB
TargetedDeconvolution.report.xml	5/19/2015 5:42 PM	XML Document	1 KB

PDF Logo File

Customize the PDF reports by replacing the shipping Agilent logo file with a desired graphic (jpeg, etc.)



2 mechanisms to create reports: via Excel or Directly (PDF reporting)

Excel

Fully supported

Uses Industry Standard Excel Plug-In

Available since initial version of MassHunter Quantitative Analysis (~10 years), 400+ templates

Excel file format can be useful for repurposing

- Word documents, Power Point Presentations

Rich content, feature-rich

PDF Reporting

Available since B.06.00 SP1

Significantly faster, especially for large data sets

Graphics are PDF direct content, virtually zero Graphics Device Interface resources consumed

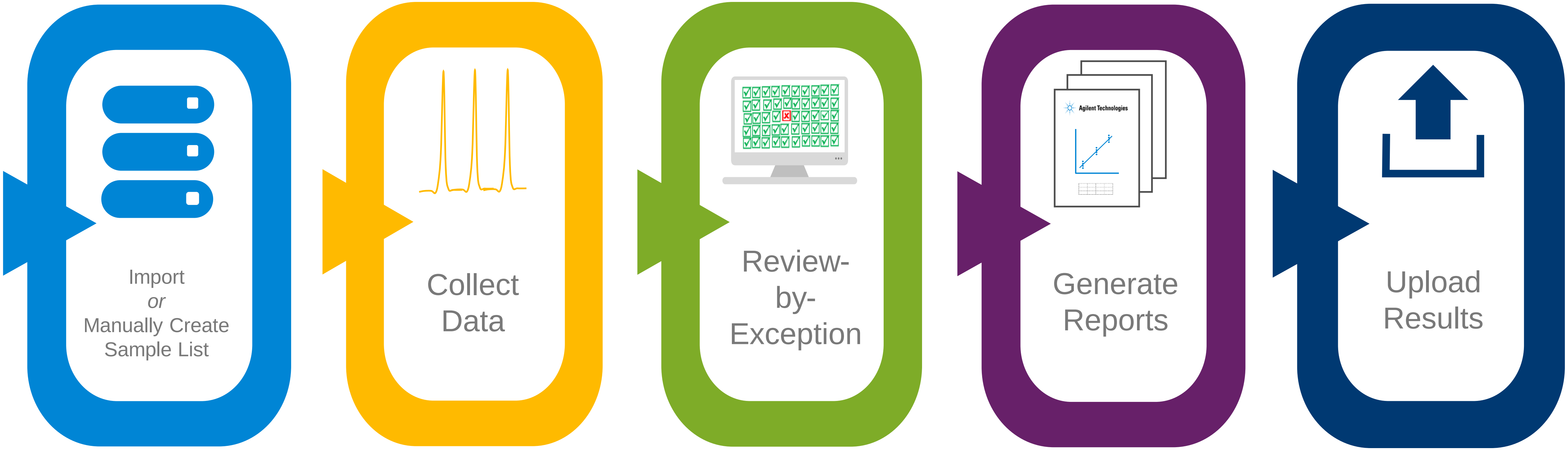
Minimum Memory Usage

Logos, labels and graphics can be customized

Based on Python programming language

Foundation for LIMS/LIS fileless integration

MassHunter Quantative Analysis Workflow



Import
or
Manually Create
Sample List

Collect
Data

Review-
by-
Exception

Generate
Reports

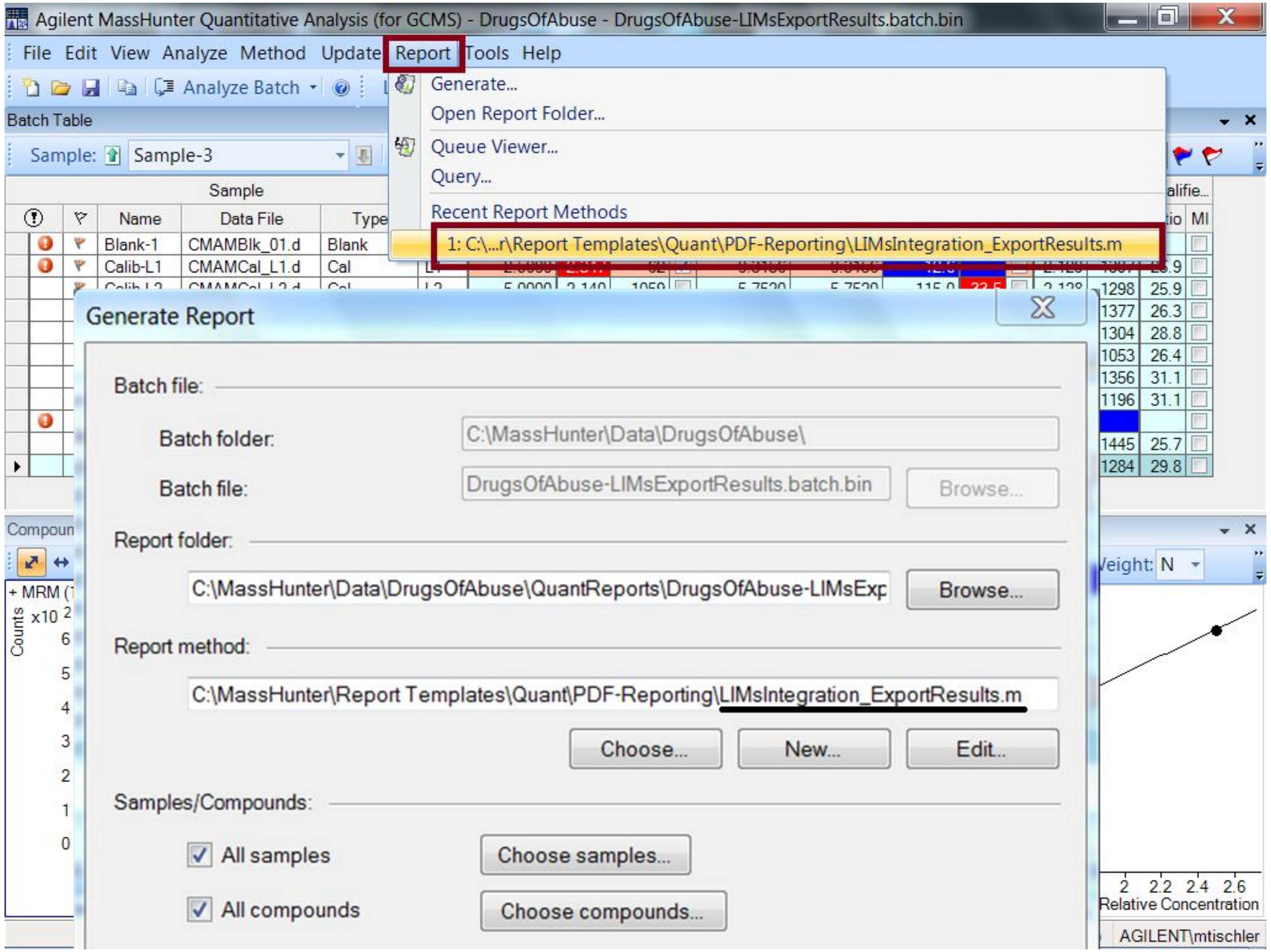
Upload
Results

Integration with LIMS/LIS/Intranet, etc.

Done via reporting method

Tutorial videos include details

- SQL Direct Insert is fileless transfer



Agilent MassHunter Quantitative Analysis (for GCMS) - DrugsOfAbuse - DrugsOfAbuse-LIMsExportResults.batch.bin

Recent Report Methods

1: C:\...r\Report Templates\Quant\PDF-Reporting\LIMsIntegration_ExportResults.m

Generate Report

Batch file:

Batch folder: C:\MassHunter\Data\DrugsOfAbuse\

Batch file: DrugsOfAbuse-LIMsExportResults.batch.bin

Report folder: C:\MassHunter\Data\DrugsOfAbuse\QuantReports\DrugsOfAbuse-LIMsExp

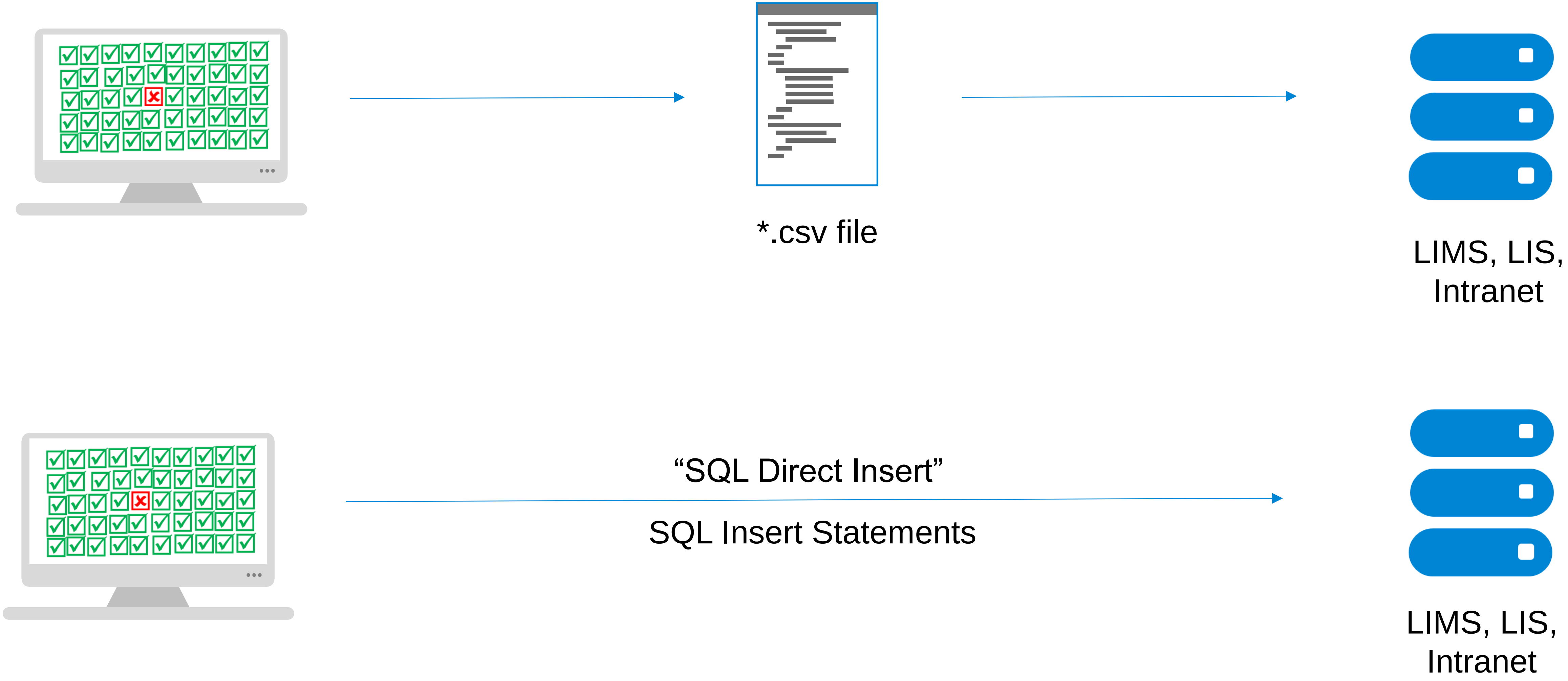
Report method: C:\MassHunter\Report Templates\Quant\PDF-Reporting\LIMsIntegration_ExportResults.m

Samples/Compounds:

☑ All samples

☑ All compounds

Uploading Results



*.csv file

LIMS, LIS,
Intranet

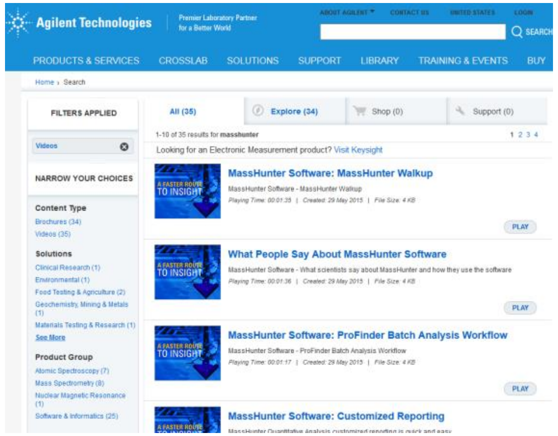
“SQL Direct Insert”

SQL Insert Statements

LIMS, LIS,
Intranet

User Community Resources Highlights

2 min videos and 30-60 min webcasts on www.agilent.com



Content Type
Brochures (34)
Videos (35)

Solutions
Clinical Research (1)
Environmental (1)
Food Testing & Agriculture (2)
Geochemistry, Mining & Metals (1)
Materials Testing & Research (1)
See More

Product Group
Atomic Spectroscopy (7)
Mass Spectrometry (8)
Nuclear Magnetic Resonance (1)
Software & Informatics (25)

1-10 of 35 results for **masshunter**

Looking for an Electronic Measurement product? Visit Keysight

MassHunter Software: MassHunter Walkup
MassHunter Software - MassHunter Walkup
Playing Time: 00:01:35 | Created: 29 May 2015 | File Size: 4 KB

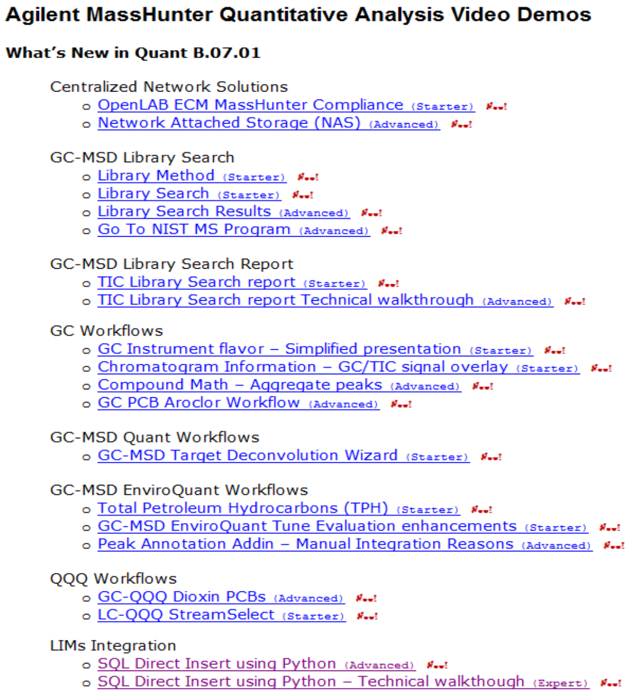
What People Say About MassHunter Software
MassHunter Software - What scientists say about MassHunter and how they use the software
Playing Time: 00:01:36 | Created: 29 May 2015 | File Size: 4 KB

MassHunter Software: ProFinder Batch Analysis Workflow
MassHunter Software - ProFinder Batch Analysis Workflow
Playing Time: 00:01:17 | Created: 29 May 2015 | File Size: 4 KB

MassHunter Software: Customized Reporting
MassHunter Quantitative Analysis customized reporting is quick and easy

Library>Videos>
Search "MassHunter"

In online Help, Videos, What's new



Agilent MassHunter Quantitative Analysis Video Demos

What's New in Quant B.07.01

Centralized Network Solutions
- OpenLAB ECM MassHunter Compliance (Starter)
- Network Attached Storage (NAS) (Advanced)

GC-MSD Library Search
- Library Method (Starter)
- Library Search (Starter)
- Library Search Results (Advanced)
- Go To NIST MS Program (Advanced)

GC-MSD Library Search Report
- TIC Library Search report (Starter)
- TIC Library Search report Technical walkthrough (Advanced)

GC Workflows
- GC Instrument flavor – Simplified presentation (Starter)
- Chromatogram Information – GC/TIC signal overlay (Starter)
- Compound Math – Aggregate peaks (Advanced)
- GC PCB Aroclor Workflow (Advanced)

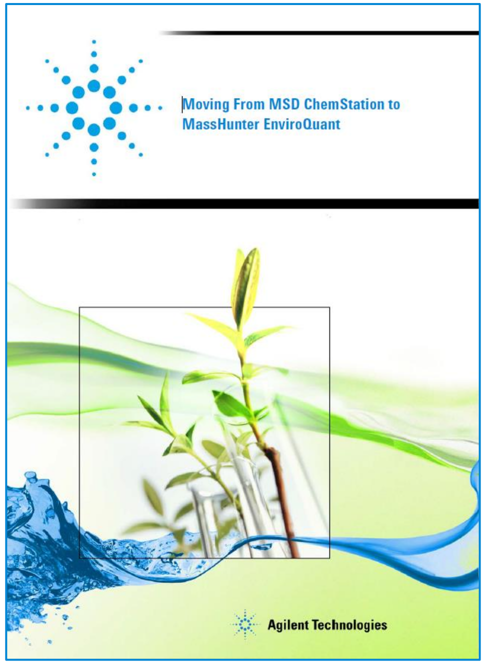
GC-MSD Quant Workflows
- GC-MSD Target Deconvolution Wizard (Starter)

GC-MSD EnviroQuant Workflows
- Total Petroleum Hydrocarbons (TPH) (Starter)
- GC-MSD EnviroQuant Tune Evaluation enhancements (Starter)
- Peak Annotation Addin – Manual Integration Reasons (Advanced)

QQQ Workflows
- GC-QQQ Dioxin PCBs (Advanced)
- LC-QQQ StreamSelect (Starter)

LIMs Integration
- SQL Direct Insert using Python (Advanced)
- SQL Direct Insert using Python – Technical walkthough (Expert)

Migration from ChemStation to MassHunter



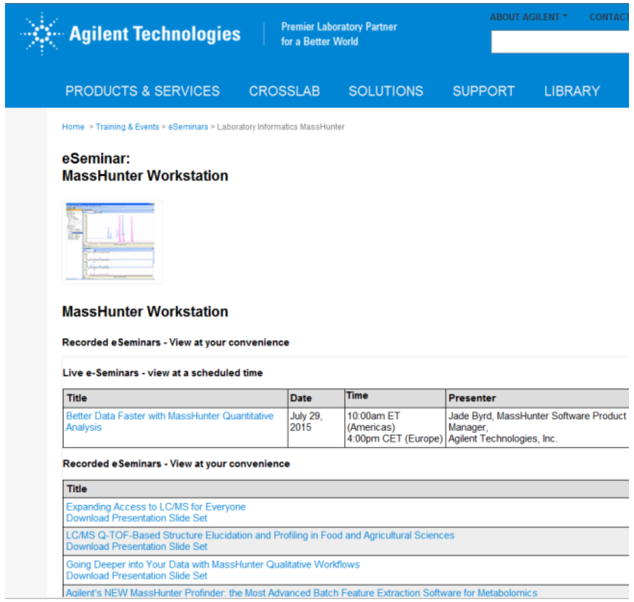
Moving From MSD ChemStation to MassHunter EnviroQuant

Agilent Technologies

Publication Part Number: G6845-90031

http://www.chem.agilent.com/Library/usermanuals/Public/EQ_ChemStation.pdf

30 min. to 1 hr. Technical Webinars



Home > Training & Events > eSeminars > Laboratory Informatics MassHunter

eSeminar:
MassHunter Workstation

MassHunter Workstation

Recorded eSeminars - View at your convenience

Live e-Seminars - view at a scheduled time

Title	Date	Time	Presenter
Better Data Faster with MassHunter Quantitative Analysis	July 29, 2015	10:00am ET (Americas) 4:00pm CET (Europe)	Jade Byrd, MassHunter Software Product Manager, Agilent Technologies, Inc.

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Feedback about MassHunter Quantitative Analysis

“We work with QC analyses that involves tracking 40 parameters, looking at a sequence of 10 samples at a time… before, we had to go sample by sample, data file by data file to evaluate the sequence… Now, with MassHunter, we have created one customized overview screen that enables us to scroll parameter by parameter all the QCs for the full sequence very quickly.”

DR. ARMAND VERBUEKEN, GC/MS USER, BAYER, ANTWERP, BELGIUM ENVIRONMENTAL TESTING LAB

“At the American games in Mexico, having an option like Compounds-at-a-Glance made it very easy to detect which compounds are positive. Also, having the capability to customize our reporting is very important because we are continuously adding new compounds to the methods and we need to incorporate them into the reporting template.”

DR. JOSEP MARCOS, LC/MS USER, THE HOSPITAL DEL MAR IN BARCELONA