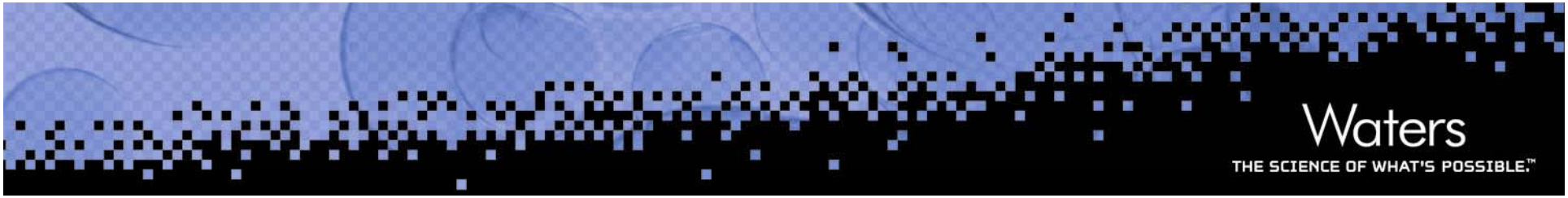

Empower 3 Software

Lauren Wood

September 2010

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Empower 3

Waters
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- Architecture
- Web based licensing
- ACQUITY improvements
- Fraction Collection
- Usability and Workflow
- Mass Spectrometry
- Method Validation Manager
- Automated Software Validation
- Designed for the Enterprise

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Empower 3 Architecture

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- Technology:
  - Oracle 11G R2 Database (64 bit)
  - Windows 2008 R2 Server Enterprise (64 bit)
  - Windows 7 Professional Operating System (64 bit)
  - Windows XP Operating System (32 bit) (clients and LAC/Es)
  - Citrix XenApp Server 6.0 running on Windows Server 2008 R2 Enterprise, 64-bit,
- Empower 3 is 32-bit app running in a 64-bit environment

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Installation

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- Operating Systems not supported
  - Windows NT
  - Windows 2000
  - Windows XP 64-bit
  - Windows 2000 Server.
- Installation will not be allowed on these OS's
- Windows Vista 32-bit, Vista 64-bit, Windows 7 32-bit and Windows Server 2003 are not supported; however, installation will be allowed on these operating systems.
- Installation on Oracle < 11.2 will be prevented; higher versions allowed
- LAC/E^{32} configurations 10 -13 supported
  - Config 10 and 11 need additional memory—2 GB minimum
  - Config 10 and 11 supported on Windows XP 32 bit only

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Installation from Previous Versions

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- Installation includes ability to perform a system object export prior to the removal of the previous version of software.
- Server installation allows you to bring the exported information into Empower 3.
  - no system object export or import offered as part of the personal installer
- System object export supported from the following versions:
  - Empower 2154 FR 3
  - Empower 2154 FR 4
  - Empower 2154 FR 5
  - Empower 1154 SP M for English
  - Empower 1154 SP SystemsQT for Japanese
  - Empower 1154 SP ISSP1 for Chinese or Korean

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Installation

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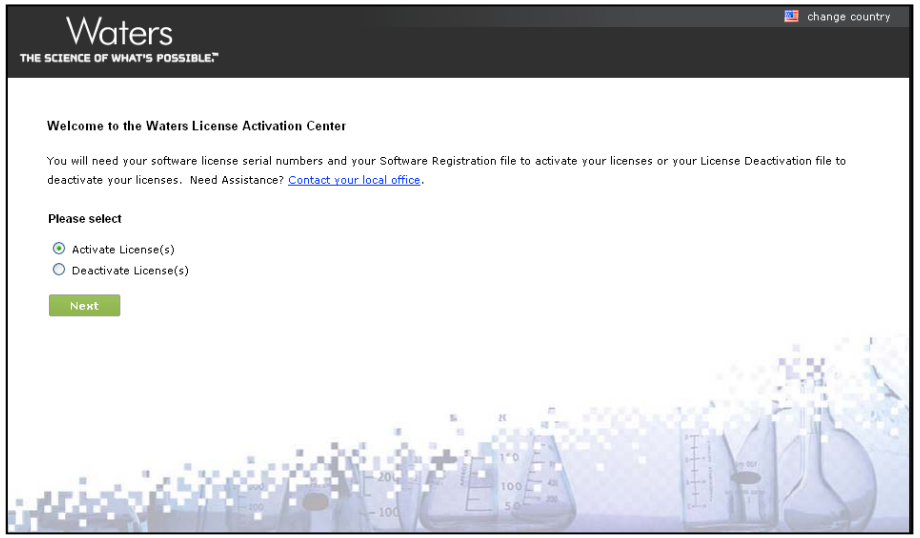
- Project restore will be supported for projects backed up in Millennium^{32} version 2.15 or higher.
- Push installations
  - Client software
  - Instrument control software
  - Waters is testing with Microsoft PSExec
  - Local + Network log file
    - Log file name = ‘computer name’ + ‘date/time stamp’
    - ‘Err’ is indicated at beginning of log file name if installation unsuccessful

Software Licensing

- Waters License Activation Center – Web
  - Used to activate and export licenses selected from order number
  - User provides contact information
  - User selects desired software serial numbers
  - License activation file is created for download
  - User executes License Wizard to activate license on computer
- Splitable user licenses
- Multi database user license



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ACQUITY eCord Information

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- Sample Set Information
  - Date
  - Sample Set Name
  - User Name
  - System Name
  - Injection Count
  - Sample Count
  - Max Pressure
  - Max Temperature
  - Sample Set Complete
- Injection information – associated with injections
  - eCord Name
  - Serial Number
  - Injection Count
- Summary information
  - Injection Count
  - Date Of First Injection
  - Date Of Last Injection
  - Sample Count
  - Maximum Pressure
  - Maximum Temperature
- Information updated after each injection
- Requires updated ICS (driver)

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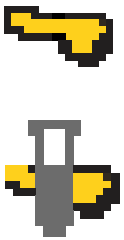
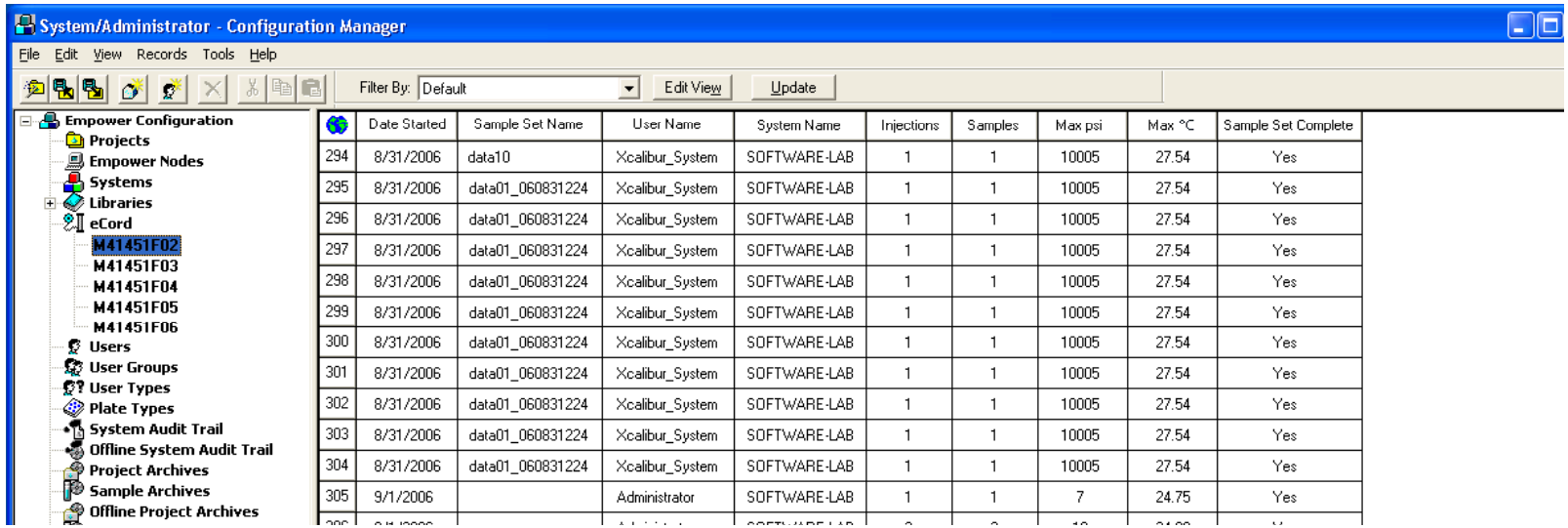
ACQUITY eCord Information

- eCord data viewed and managed in Configuration Manager
  - eCord Summary Table
  - eCord Sample Sets table
- eCords added automatically when data is acquired using system containing eCord
- Enumerated custom fields called Column Name and Column Serial Number (for non-ACQUITY systems)





	Date Started	Sample Set Name	User Name	System Name	Injections	Samples	Max psi	Max °C	Sample Set Complete
294	8/31/2006	data10	Xcalibur_System	SOFTWARE-LAB	1	1	10005	27.54	Yes
295	8/31/2006	data01_060831224	Xcalibur_System	SOFTWARE-LAB	1	1	10005	27.54	Yes
296	8/31/2006	data01_060831224	Xcalibur_System	SOFTWARE-LAB	1	1	10005	27.54	Yes
297	8/31/2006	data01_060831224	Xcalibur_System	SOFTWARE-LAB	1	1	10005	27.54	Yes
298	8/31/2006	data01_060831224	Xcalibur_System	SOFTWARE-LAB	1	1	10005	27.54	Yes
299	8/31/2006	data01_060831224	Xcalibur_System	SOFTWARE-LAB	1	1	10005	27.54	Yes
300	8/31/2006	data01_060831224	Xcalibur_System	SOFTWARE-LAB	1	1	10005	27.54	Yes
301	8/31/2006	data01_060831224	Xcalibur_System	SOFTWARE-LAB	1	1	10005	27.54	Yes
302	8/31/2006	data01_060831224	Xcalibur_System	SOFTWARE-LAB	1	1	10005	27.54	Yes
303	8/31/2006	data01_060831224	Xcalibur_System	SOFTWARE-LAB	1	1	10005	27.54	Yes
304	8/31/2006	data01_060831224	Xcalibur_System	SOFTWARE-LAB	1	1	10005	27.54	Yes
305	9/1/2006		Administrator	SOFTWARE-LAB	1	1	7	24.75	Yes

ACQUITY Injection Modes

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- **Run Samples and QuickStart**
- **Full Loop Mode**
  - Injection volume field automatically filled in with the loop volume
  - Field not editable
- **Partial Loop Mode / with Needle Overfill**
  - Injection volume must be within the valid injectable volume range defined by the instrument
  - Editable field

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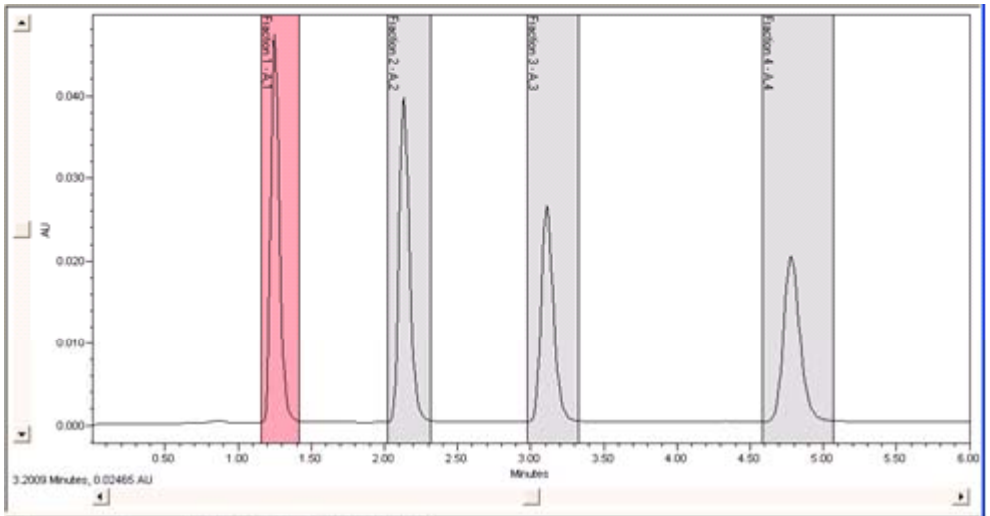
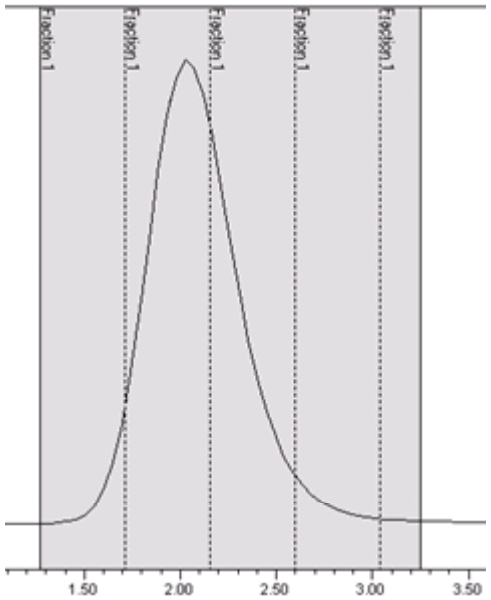
- WFC III control in Empower 2
- Enhancements in Empower 3
  - Fraction annotations on chromatogram
  - Fraction table
  - Fraction tab in Project window



	Name	Location	Fraction Index	Location Index	Start Time (min)	End Time (min)
1	Fraction 1	A,1	1	1	1.158	1.417
2	Fraction 2	A,2	2	1	2.025	2.3 7
3	Fraction 3	A,3	3	1	2.975	3.325
4	Fraction 4	A,4	4	1	4.583	5.067

2D Channels | Fractions | Peaks



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Usability

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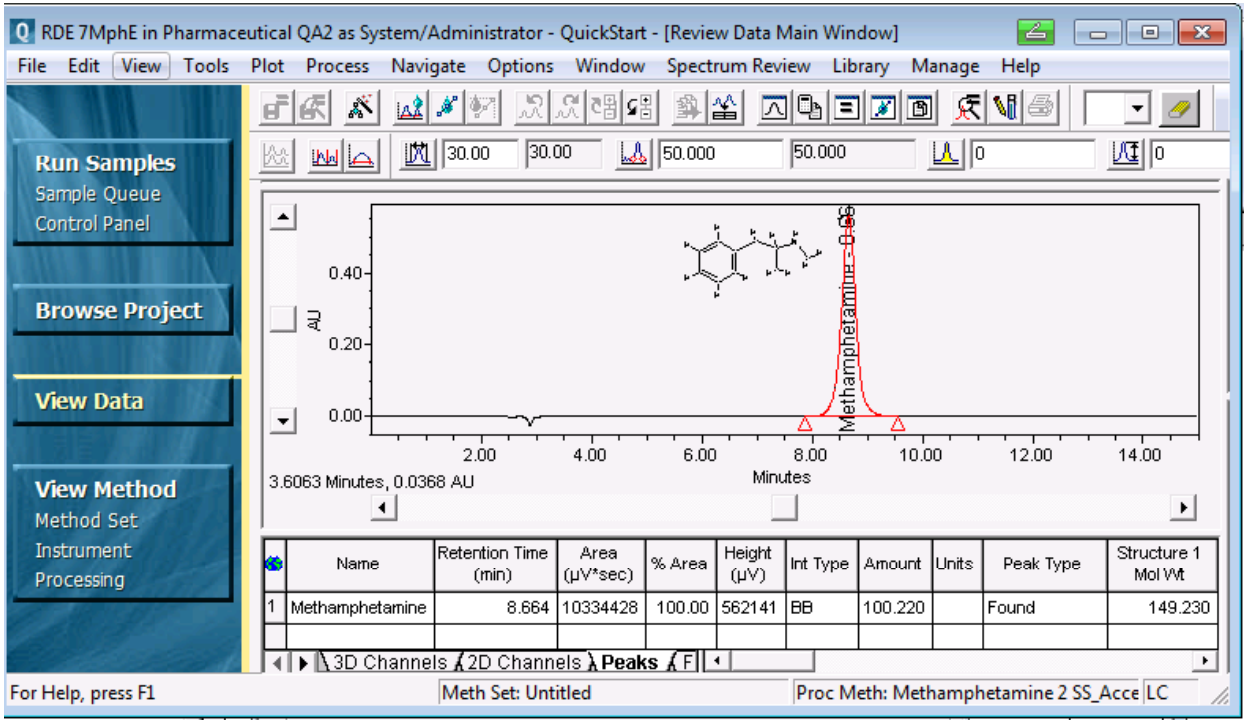
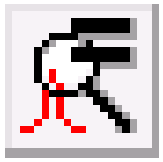
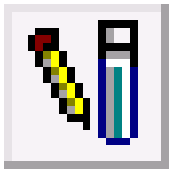
Navigate from Review to….





▪ Preview

▪Save and Preview



▪Alter Sample

▪Run Samples

Navigate tree using arrow keys ↑↓

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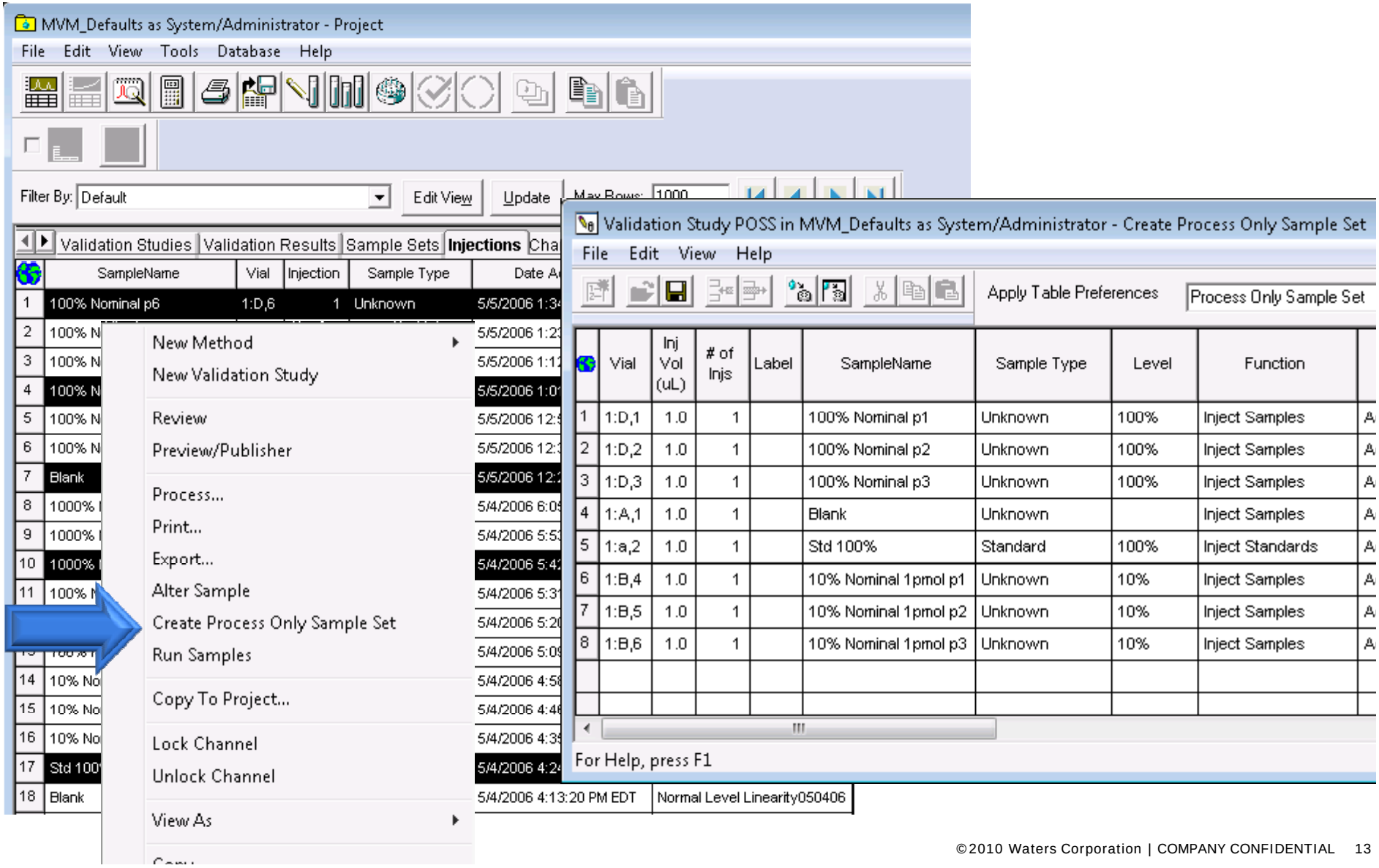
Process Only Sample Sets



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Process Only Sample Sets

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- Allows combining disparate injections into a sample set post-acquisition
  - Allows flexibility in processing
  - Allows combination for use of individual injections in MVM
  - Allows combination for use in Dissolution/CU multi-phase studies
- Privilege called Manage Process Only Sample Set
- Fully audit trailed
- Creating and editing as in Alter Sample -is similar to altering a regular sample set.

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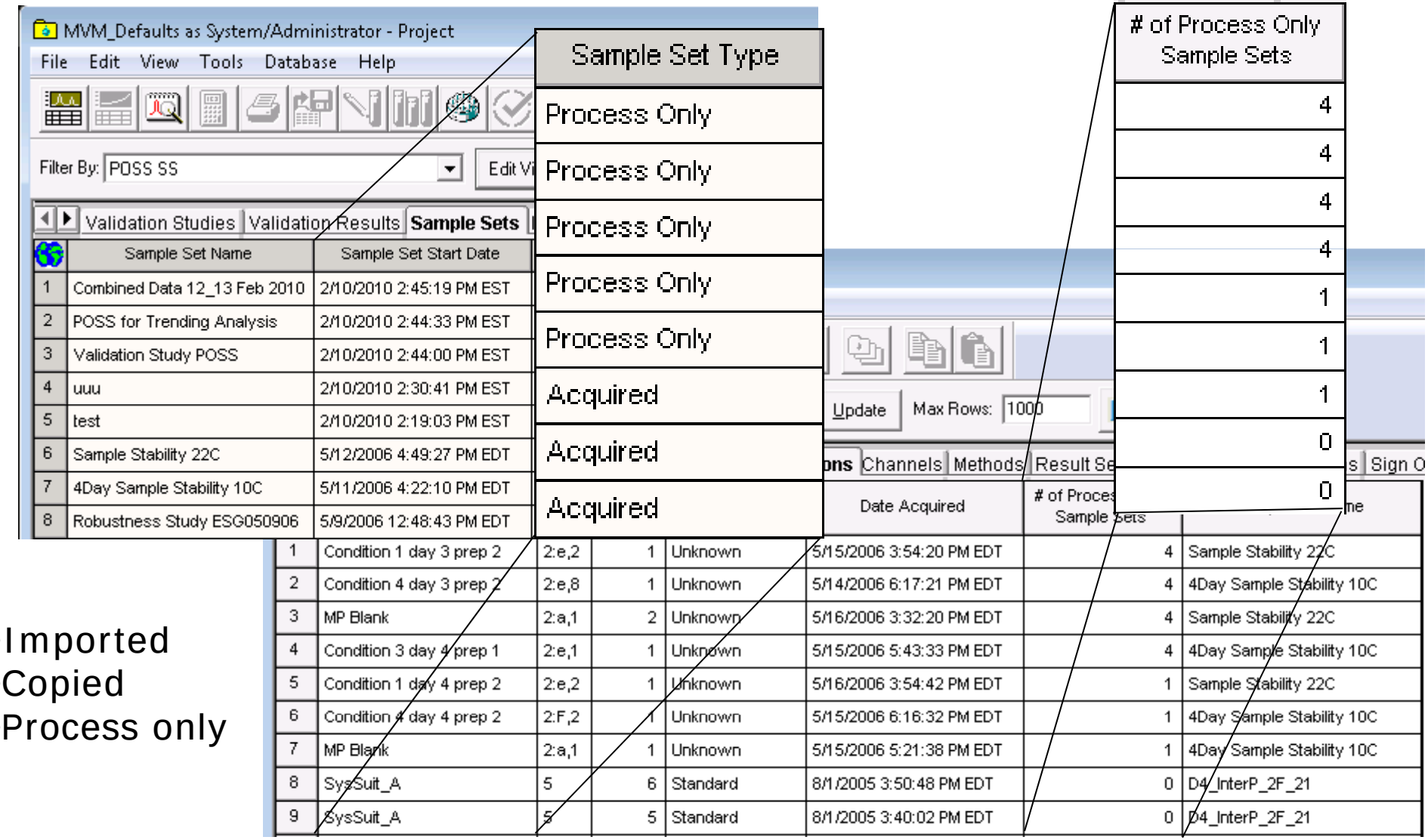
Process Only Sample Sets



- Imported
- Copied
- Process only

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Usability

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- Project integrity errors won't stop batch project backup/restore
  - Log file is generated to document errors
  - Time zone and database update request also won't stop backup
- Multiple application windows locked due to timeout
  - Unlock once to unlock all
  - Does not pertain to 6-button window
- Run Samples Control Panel Position saved as preference

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Usability

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- View Message Center for All Users privilege
  - Allows granularity to specify users that see all messages or only their own
- ApexTrack - Use appropriate peak width for USP Plate Count USP Resolution and Relative Resolution determination
  - Values dependant on inflection points → Width@Tangent
  - Incorrect peak width parameter could over smooth data in previous versions
  - Software will recalculate peak's inflection points using a peak width that is appropriate (correct) for the peak instead of the possibly inappropriate peak width in the method
  - Affects peaks using PW outside of 2X Auto-PeakWidth range
  - No more message regarding "Inappropriate Peak Width"

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EP / JP / USP Signal to Noise

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The signal-to-noise ratio (S/N) is a useful system suitability parameter. The S/N is calculated as follows:

$$S/N = 2H/h$$

where H is the height of the peak measured from the peak apex to a baseline extrapolated over a distance ≥5 times the peak width at its half-height; and h is the difference between the largest and smallest noise values observed over a distance ≥5 times the width at the half-height of the peak and, if possible, situated equally around the peak of interest after the injection or application of a blank (see *Figure 5*).

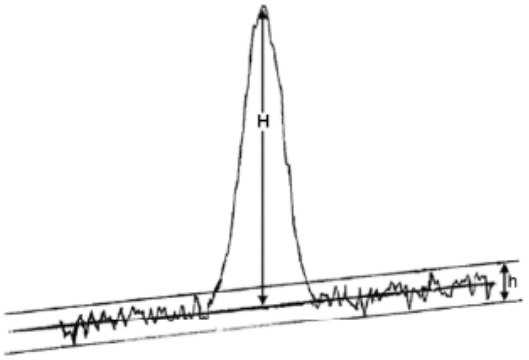
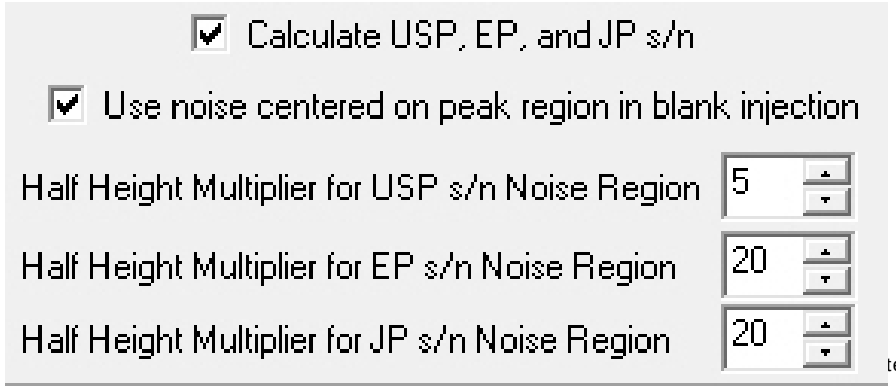


Figure 5. Noise and chromatographic peak, components of the S/N ratio.



EP / JP / USP Signal to Noise

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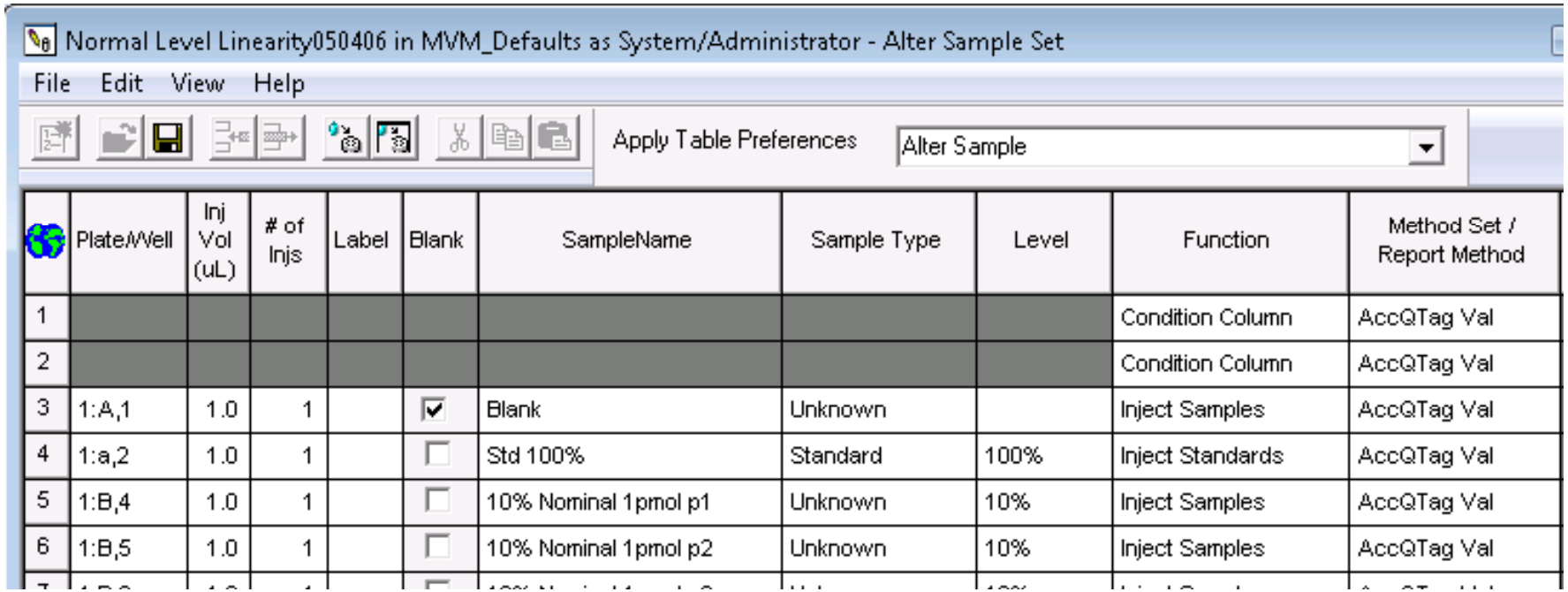
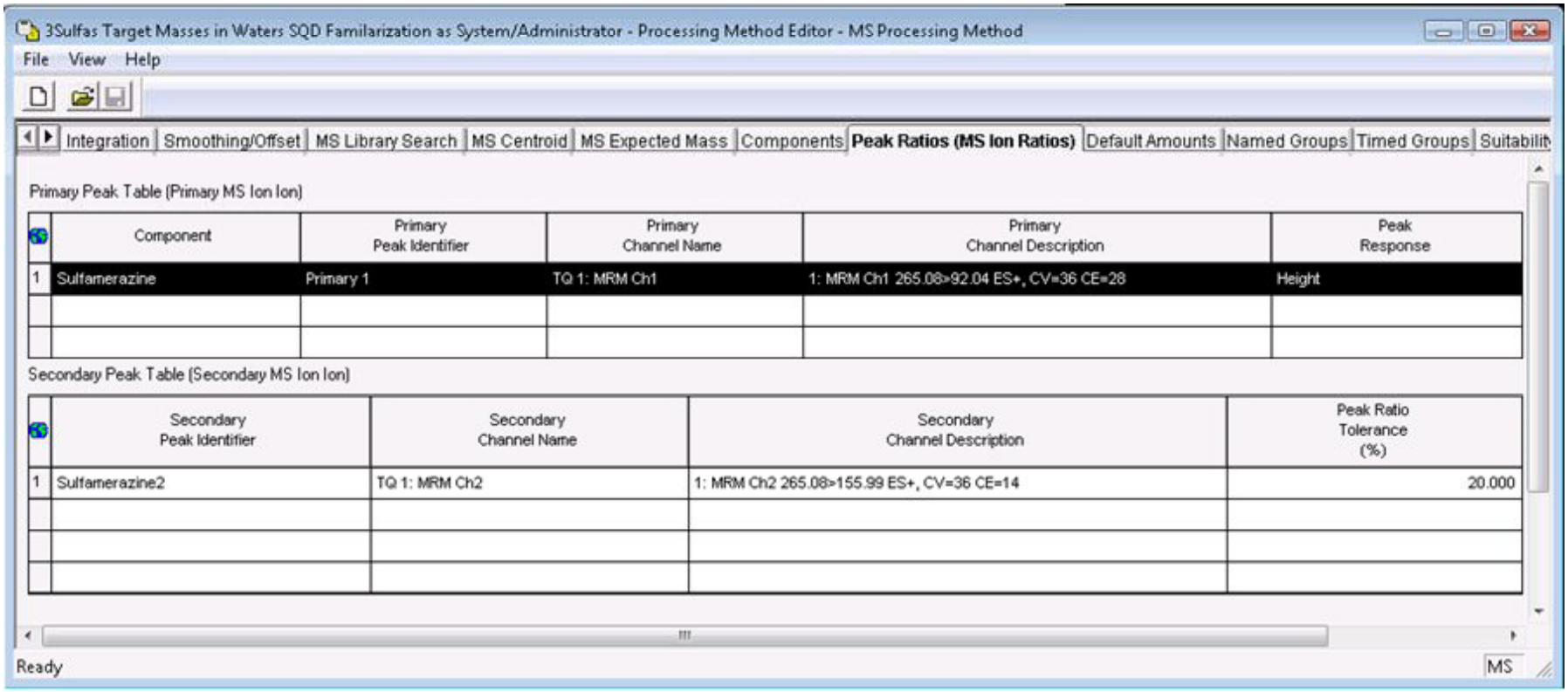
- Allows determination of noise within a blank injection centered on the peak region
- Allows user to specify a noise segment based on peak width at half height:
  - USP Half Height Multiplier for Noise Region
  - EP Half Height Multiplier for Noise Region
  - JP Half Height Multiplier for Noise Region



	Plate/Well	Inj Vol (uL)	# of Injs	Label	Blank	SampleName	Sample Type	Level	Function	Method Set / Report Method
1									Condition Column	AccQTag Val
2									Condition Column	AccQTag Val
3	1:A,1	1.0	1		☑	Blank	Unknown		Inject Samples	AccQTag Val
4	1:a,2	1.0	1		☐	Std 100%	Standard	100%	Inject Standards	AccQTag Val
5	1:B,4	1.0	1		☐	10% Nominal 1pmol p1	Unknown	10%	Inject Samples	AccQTag Val
6	1:B,5	1.0	1		☐	10% Nominal 1pmol p2	Unknown	10%	Inject Samples	AccQTag Val

MS Ion Ratios + Acceptance Tolerance

- For defensible compound confirmation
- Area or Height ratio of 1^0 Channel : 2^0 Channel (1 – 4) in same injection
- Acceptance tolerance on result as compared to a reference injection
- Failed values are faulted



MS Target Masses

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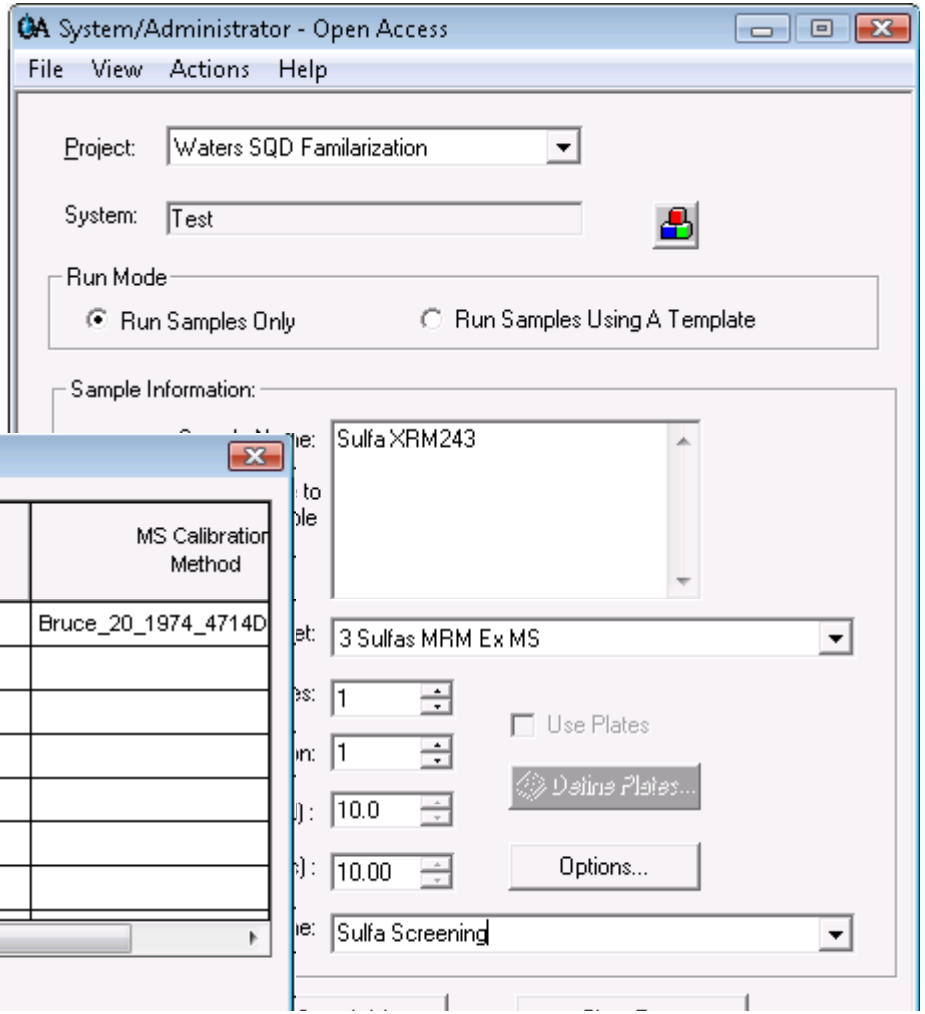
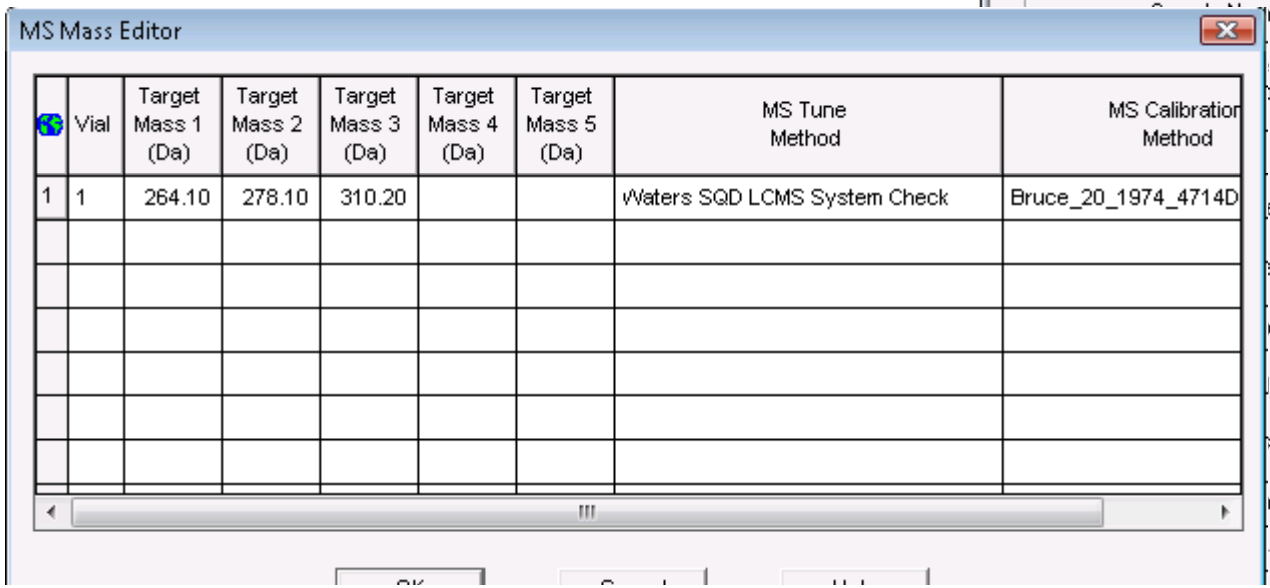
- Open Access, Run Samples, QuickStart, Alter Sample
- Specify up to 5 base monoisotopic masses in sample table (not processing method)
- Possible adducts entered in PM
- Obtain Yes/No answer as to whether the target mass is present in sample

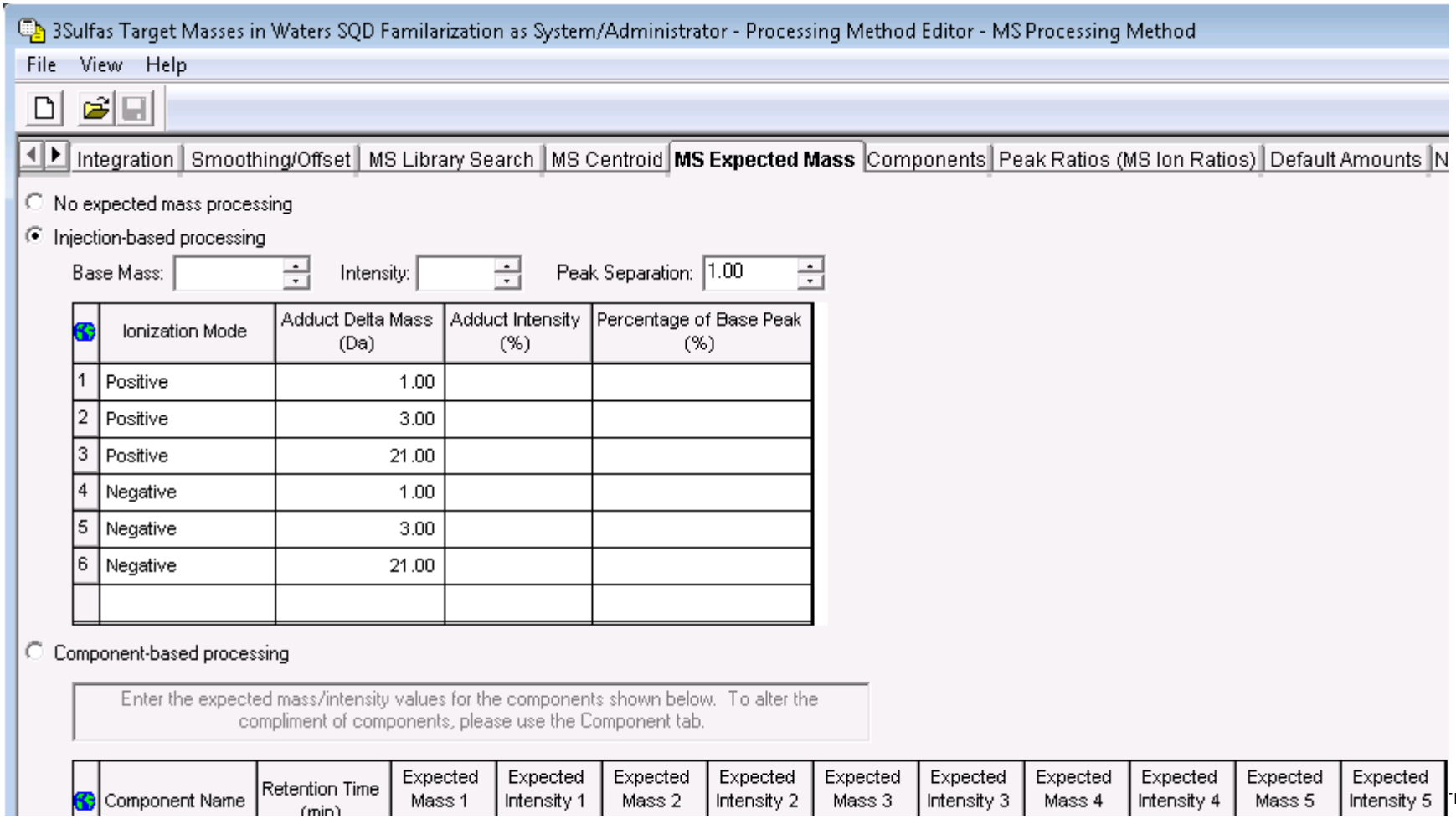




	Vial	Target Mass 1 (Da)	Target Mass 2 (Da)	Target Mass 3 (Da)	Target Mass 4 (Da)	Target Mass 5 (Da)	MS Tune Method	MS Calibration Method
1	1	264.10	278.10	310.20			Waters SQD LCMS System Check	Bruce_20_1974_4714D

MS Target Masses

- Masses specified in Run Samples supersede the one in the processing method



	Ionization Mode	Adduct Delta Mass (Da)	Adduct Intensity (%)	Percentage of Base Peak (%)
1	Positive	1.00		
2	Positive	3.00		
3	Positive	21.00		
4	Negative	1.00		
5	Negative	3.00		
6	Negative	21.00		

Component Name	Retention Time (min)	Expected Mass 1	Expected Intensity 1	Expected Mass 2	Expected Intensity 2	Expected Mass 3	Expected Intensity 3	Expected Mass 4	Expected Intensity 4	Expected Mass 5	Expected Intensity 5

MVM : SFSTP Calculations

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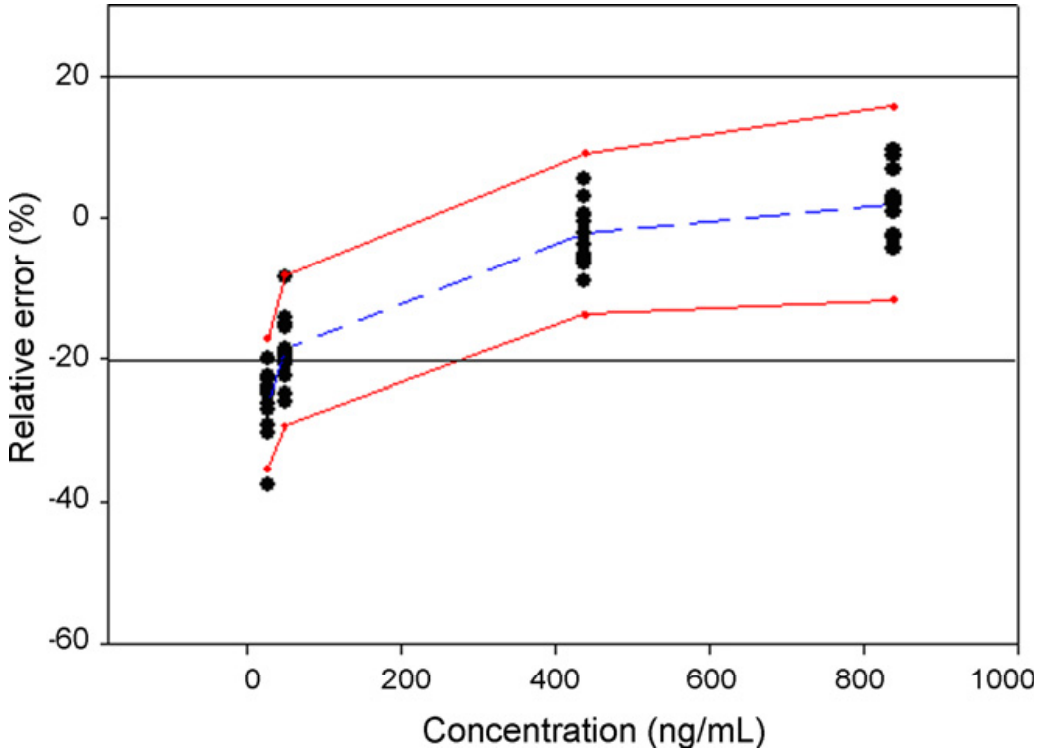
- Accuracy Total Error
  - Sums intermediate precision and bias
  - % Total Error
  - % Relative Error
  - % Relative Error Mean
  - Tolerance Interval
  - Upper/Lower Limit of Quantitation

- Accuracy Profile Plot
- % Relative Error vs. X Value



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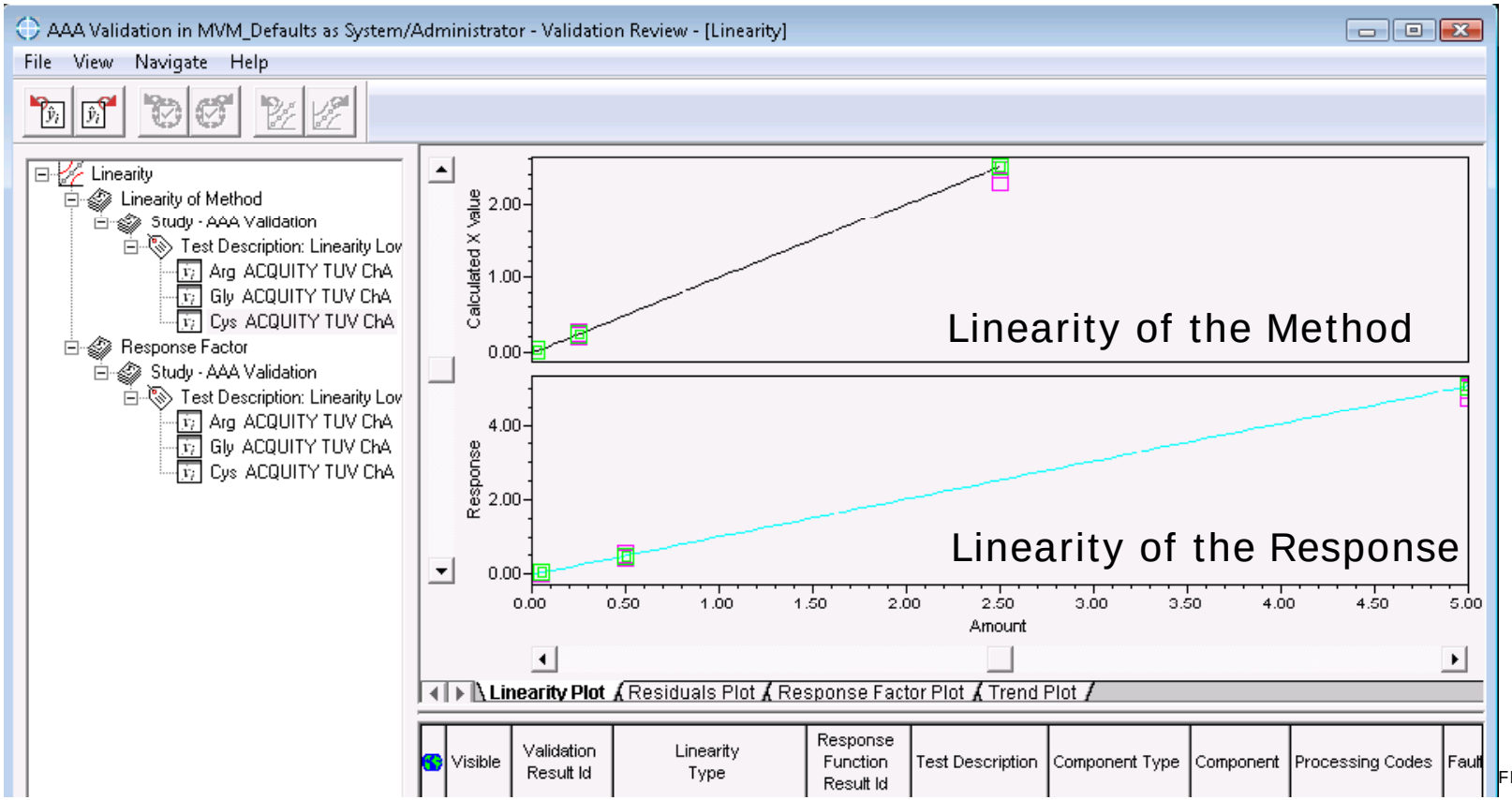
MVM – Linearity of the Method

- Linearity of the Response (current) – Response vs. Amount/Concentration
- Linearity of the Method - Calculated value (from linearity of response) vs. Amount/Concentration



Validation Services

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- Validation: barrier to adopting new software & updates
- Leverage ESS Proven record of success in > 40 Empower customers + 10 years validation experience
- Automation of existing test execution
  - Estimates suggest that automating tests will take half the time for execution
- Complementary service to Connections AQT and SystemsQT

SystemsQT

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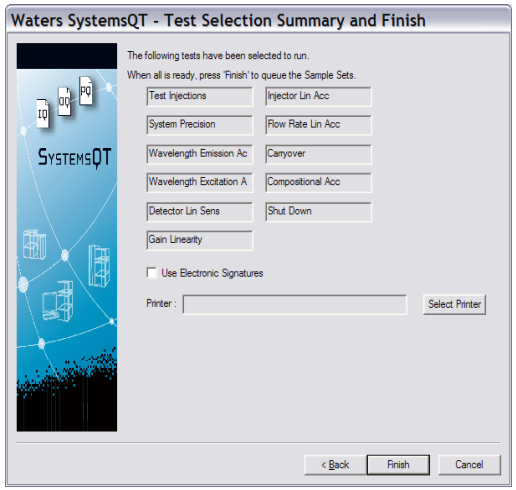
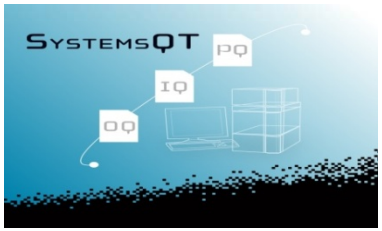
- Service offering for new chromatographic system qualification tool for system level test
- Integrated Empower 3 Software
  - Launch SystemsQT Wizard from Run Samples to Qualify System
- Wizard guides user through the system qualification setup
- Each system configuration includes an Empower project with predefined sample sets, calculations and reports





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Supported Configuration with SystemsQT

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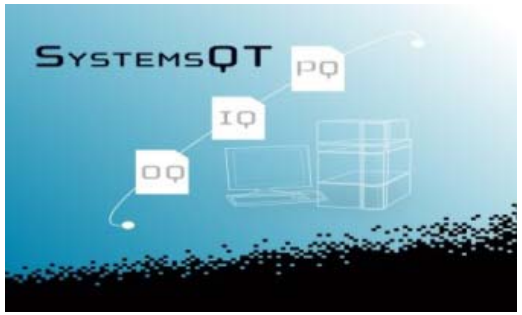
- All ACQUITY Configurations
  - All modules including the ACQUITY Fluorescence Detector, ACQUITY Photodiode Array Detector, ACQUITY Tunable UV Detector, ACQUITY Evaporative Light Scattering Detector, ACQUITY SQD single quadrupole Mass Detector and ACQUITY TQD tandem quadrupole Mass Detector
- All Alliance 2695/2795 Configurations
  - Including the Waters UV/Visible Detectors, Waters PDA Detector, Waters FLR Detector, Waters RI Detectors, Waters 3100 SQ and TQD tandem quadrupole Mass Detectors
- Modular HPLC Systems
  - Including 1515/1525 Pumps, 2707 injector and RI/UV detectors
- Agilent LC Configurations
  - Including UV, DAD, RI and FLR Detectors
- Agilent GC Configurations
  - 7890, 6890, 6850 and G1888 HS



Fusion Method Development Software with ACQUITY UPLC

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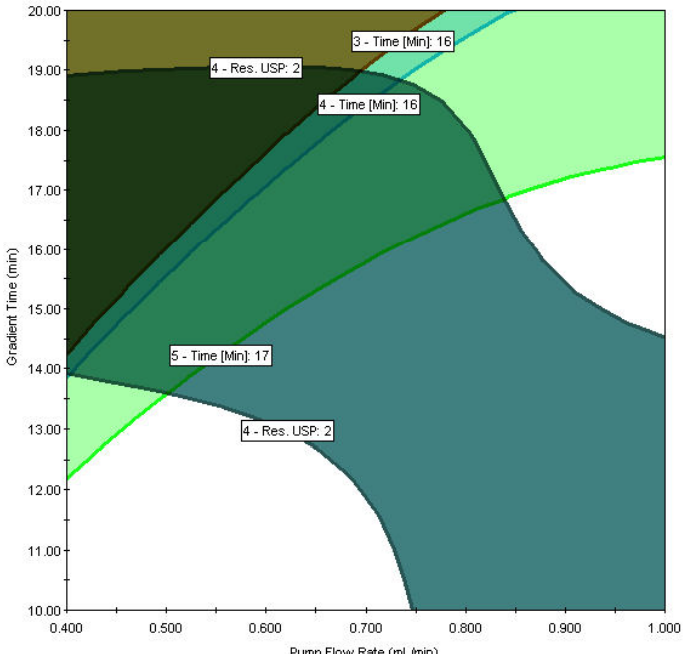
- Reduces method development time from weeks to days
- Create and builds statistically valid experimental designs
- Predict optimal conditions for the process under study
- Builds robustness in for the long-term viability and transferability of the method
- Generates a statistically valid design space
  - Characterizes the impact of chromatographic parameters on separation performance
  - Eliminates/reduces method re-validation re-work
  - Aligned with QbD guidelines
- Increased efficiency and confidence that methods will Validate and transfer



S-Matrix®

Fusion Method Development Software with ACQUITY UPLC

Waters
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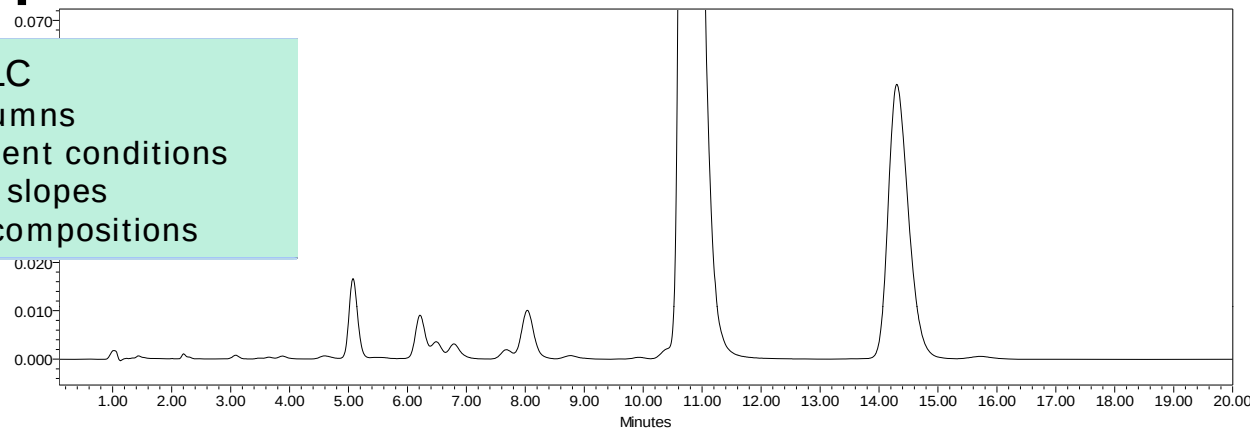
Original Approach

HPLC
10 columns
Isocratic & gradient conditions
Gradient slopes
Mobile phase compositions

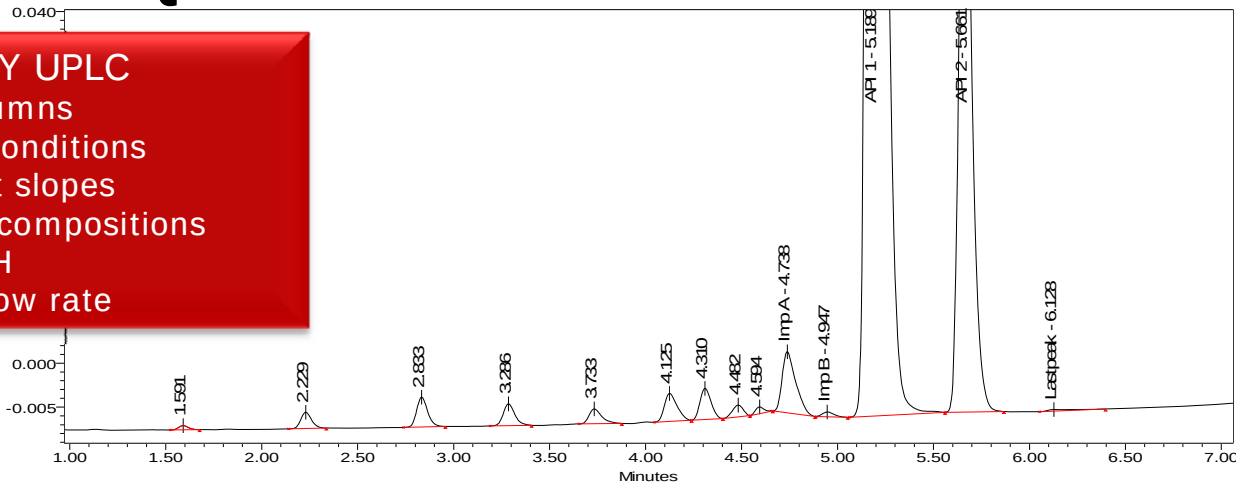
45 days



Fusion with ACQUITY UPLC®

ACQUITY UPLC
3 columns
Gradient conditions
Gradient slopes
Mobile phase compositions
pH
Pump flow rate

2 days



S-Matrix®

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Empower 3 Software

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- Tools for the Chemist
  - New Instrument Control
  - Usability features
  - Option enhancement
  - Process only Sample Sets
- Tools for the Lab Managers and Administrators
  - Help with Deployment in complex architectures
  - Simpler License management
  - Easier Global deployment
  - Tools to streamline the software validation process

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Discussion

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