Empower 3 Software

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September 2010
- Architecture
- Web based licensing
- ACQUITY improvements
- Fraction Collection
- Usability and Workflow
- Mass Spectrometry
- Method Validation Manager
- Automated Software Validation
- Designed for the Enterprise
Empower 3 Architecture

- **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
Installation

- Operating Systems not supported
  - Windows NT
  - Windows 2000
  - Windows XP 64-bit

- 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$E^{32}$ 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
Installation from Previous Versions

- 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
- Project restore will be supported for projects backed up in Millennium\textsuperscript{32} version 2.15 or higher.
- Push installations
  - Client software
  - Instrument control software
  - Waters is testing with Microsoft PSEexec
  - 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
ACQUITY eCord Information

- 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)
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)
ACQUITY Injection Modes

- **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
- WFC III control in Empower 2
- Enhancements in Empower 3
  - Fraction annotations on chromatogram
  - Fraction table
  - Fraction tab in Project window
Navigate from Review to....

- Preview
- Save and Preview
- Alter Sample
- Run Samples

Navigate tree using arrow keys ↑↓
Process Only Sample Sets

- 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.
### Process Only Sample Sets

#### Sample Set Type
- Process Only
- Process Only
- Process Only
- Process Only
- Acquired
- Acquired
- Acquired

#### # of Process Only Sample Sets

<table>
<thead>
<tr>
<th>Sample Set Name</th>
<th>Sample Set Start Date</th>
<th>Date Acquired</th>
<th># of Process Only Sample Sets</th>
</tr>
</thead>
<tbody>
<tr>
<td>POSS for Trending Analysis</td>
<td>2/1/2010 2:44:33 PM EST</td>
<td>5/14/2006 6:17:21 PM EDT</td>
<td>4</td>
</tr>
<tr>
<td>Validation Study POSS</td>
<td>2/1/2010 2:44:00 PM EST</td>
<td>5/15/2006 3:54:20 PM EDT</td>
<td>4</td>
</tr>
</tbody>
</table>

### Important Notes
- Imported
- Copied
- Process only
- 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
- **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”
The signal-to-noise ratio (S/N) is a useful system suitability parameter. The S/N is calculated as follows:

\[ \text{S/N} = \frac{2H}{h} \]

where \( H \) is the height of the peak measured from the peak apex to a baseline extrapolated over a distance \( \geq 5 \) times the peak width at its half-height; and \( h \) is the difference between the largest and smallest noise values observed over a distance \( \geq 5 \) 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.

- [ ] Calculate USP, EP, and JP s/n
- [ ] Use noise centered on peak region in blank injection

| Half Height Multiplier for USP s/n Noise Region | 5 |
| Half Height Multiplier for EP s/n Noise Region | 20 |
| Half Height Multiplier for JP s/n Noise Region | 20 |
EP/JP/USP Signal to Noise

- 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
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
- 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
Masses specified in Run Samples supersede the one in the processing method.
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
- Linearity of the Response (current) – Response vs. Amount/Concentration
- Linearity of the Method - Calculated value (from linearity of response) vs. Amount/Concentration
Validation Services

- 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
- 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
Supported Configuration with SystemsQT

- **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

- 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
**Fusion Method Development Software with ACQUITY UPLC**

**Original Approach**

<table>
<thead>
<tr>
<th>HPLC</th>
</tr>
</thead>
<tbody>
<tr>
<td>10 columns</td>
</tr>
<tr>
<td>Isocratic &amp; gradient conditions</td>
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<tr>
<td>Gradient slopes</td>
</tr>
<tr>
<td>Mobile phase compositions</td>
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</tbody>
</table>

**Fusion with ACQUITY UPLC®**

<table>
<thead>
<tr>
<th>ACQUITY UPLC</th>
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</thead>
<tbody>
<tr>
<td>3 columns</td>
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<tr>
<td>Gradient conditions</td>
</tr>
<tr>
<td>Gradient slopes</td>
</tr>
<tr>
<td>Mobile phase compositions</td>
</tr>
<tr>
<td>pH</td>
</tr>
<tr>
<td>Pump flow rate</td>
</tr>
</tbody>
</table>

45 days

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Empower 3 Software

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