

EZChrom Elite

What's New in EZChrom Elite 3.3.2 Service Pack 1



Agilent Technologies

Notices

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Using This Guide

Introduction

This Document lists the design changes introduced with Service Pack 1 for EZChrom Elite 3.3.2. It describes new functionality that might differ from the previous behavior as described in the online help.

Who Should Read This Guide?

This document is designed for the end user or system administrator who will use or manage the Agilent EZChrom Elite system.

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List of Changes

Data Analysis

1) Additional Custom Parameter to support European Pharmacopeia Updates

EZChrom Elite 3.3.2: The following European Pharmacopeia updated calculations were not supported within EZChrom.

Peak-to-Valley Ratio

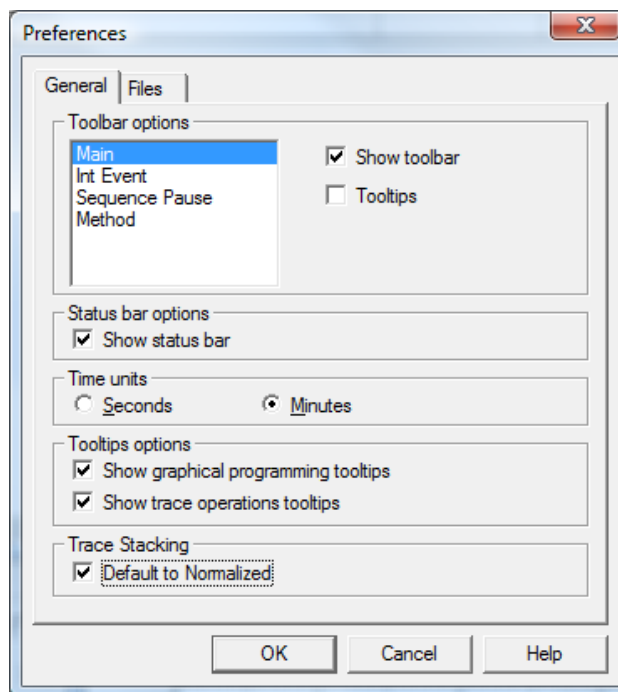
Signal-to-Noise Ratio

EZChrom Elite 3.3.2 SP1: New custom parameters have been created to provide full support of these calculations. Please refer to the online help topic equations “European Pharmacopoeia Signal to Noise” and “Peak-to-Valley Ratio” for details on enabling and using these. Once the custom parameter is turned on a method, the reporting variables become available for reports and annotations.

2) Additional Preference Option to pre-define signal Stacking normalization

EZChrom Elite 3.3.2: New traces are always normalized to the first chromatogram by default.

EZChrom Elite 3.3.2 SP1: A new option has been added under View/preferences that allow the user to disable automatic normalization to the first chromatogram. This user setting is retained on a per-instrument per-user basis.



Workflow Improvements

Import/Export Enhancements for Interfacing to other Systems

3) Sequence Import Enhancements

EZChrom Elite 3.3.2: The system currently does not provide the capabilities to import “Custom Parameters” and “Concentration Overrides” in a batch sequence.

EZChrom Elite 3.3.2 SP1: Functionality has been added to the import of ASCII sequence templates. With this service pack users will be able to define methods at import time and import ASCII sequences that contain custom parameter and concentration override information.

See the EZChrom Elite help page “*ASCII file formats*” for details on sequence import.

1. New import keys for custom parameters are defined as given below:

CUSTOMPARAMPEAK = a,b,c,d

CUSTOMPARAMSYS = c, d

Where,

- **a:**
 - Detector Trace Name – Full detector trace name to which the custom parameters shall be applied. Comma separators are not permitted in the parameter field. If the trace name contains comma (“,”) separator, specify the trace name till the separator.
For example, if the Trace Name is “VWD: Signal A, 250 nm”, the parameter field in ASCII should be “VWD: Signal A”
 - Detector Trace Number – Trace number displayed in the Channel combo box on the instrument client for the appropriate detector. The trace number should be specified in notation given below.

Notation for Trace Number: “[**num**]” where num refers to trace number.

- **b:** Compound ID – Peak name given in the peak table of the specified method, this value is case-sensitive.
- **c:** Custom Parameter ID – Custom parameter name from the specified method, this value is case-sensitive.
- **d:** Parameter Value – Supports both String and Number values.

2. New import keys for concentration overrides are defined as given below:

CONCOVERRIDE = a,b,c,d

Where,

- **a:**

- Detector Trace Name – Full detector trace name to which the custom parameters shall be applied. Comma separators are not permitted in the parameter field. If the trace name contains comma (“,”) separator, specify the trace name till the separator.
For example, if the Trace Name is “VWD: Signal A, 250 nm”, the parameter field in ASCII should be “VWD: Signal A”
- Detector Trace Number – Trace number displayed in the Channel combo box on the instrument client for the appropriate detector. The trace number should be specified in notation given below.
Notation for Trace Number: “[num]” where num refers to trace number.
- **b:** Concentration type – “P” for peak and “G” for group
For group type, concentration override applies only for calibrated range; override values are not applicable for uncalibrated range or named peaks.
- **c:** Compound ID – Peak/Group name given in the peak table of the specified method, this value is case-sensitive.
- **d:** Concentration override value to be applied

3. New keys to prompt Method selection are defined as given below:

RECORD = a,b,c,d,e,f,g,h,I,j,k,l,m,n,o,p,q,r,s,t,u

Where,

- **b:** Method Name (63 characters maximum)
 - To allow the user select the method while importing the batch file, the following notation should be specified instead of the method path.

Notation to prompt for method selection: “[?]”
 - In case the prompt notation is used, the batch file should be saved for further usage like acquisition, reprocessing ...etc.
 - Any subsequent record with PROMPT NOTATION will use the user selected method.

LIMS EXPORT: Following peak parameters in Advanced Report from both Sequence and Data File sources are not exported.

Peak ID: Assigned Peak number in the Peak/Group table

Raw Amount: On Column amount without Multiplier/Dilutor

Flag for ISTD Peak: A parameter to identify the current peak as either ISTD or not.

Curve Fit Parameters: Display curve fit parameters used in calculating Calibration Curve.

Run Type: Run type defined for a particular record in sequence file (SEQUENCE ONLY)

4) Advanced Report Enhancements

EZChrom Elite 3.3.2: Several parameters available in Advanced Reports are not available for export.

EZChrom Elite 3.3.2 SP1: Support has been added to allow export of the following new parameters as available in Advanced Reports.

Peak ID:

An ID value is already assigned for each peak added to the peak table. This value is not currently exportable. A new peak result entry (NAMEDPEAKID) has been created. The NAMEDPEAKID entry is accessible as follows:

Access Code: PEAK.NAMEDPEAKID
 Function: PEAK.NAMEDPEAKID ("R1","T1","P1; 3")

Raw Amount:

Raw amount calculation for a peak. A new peak result entry (RAWAMOUNT) has been created that contains the calculated value. The calculation is [Response in Area] * [Response Factor without multiplier/dilutor]. The RAWAMOUNT entry is accessible as follows:

Access Code: PEAK.RAWAMOUNT
 Function: PEAK. RAWAMOUNT ("R1","T1","P1; 3")

Flag for ISTD:

Each peak in the peak table can be assigned as an ISTD. The peak table list the corresponding information about ISTD peaks but was not available for reporting. A new peak result entry (ISTDPEAK) has been created to be used for reporting purpose. The ISTDPEAK entry is accessible as follows:

Access Code: PEAK.ISTDPEAK
 Function: PEAK. ISTDPEAK ("R1","T1","P1; 3")
 Result: "ISTD PEAK" or {Empty string}

Curve Fit Parameters:

In Review Peak Calibration, the curve fit parameters are displayed, but there were not exported. A bunch of peak result entries shall be created to display the parameters used in calibration calculation.

Fit Quality: If curve type is average, FitQuality would contain RSD of the Average, otherwise it would be goodness fit (r^2).

The peak result entries are accessible as follows:

Access Code: PEAK.CURVETYPE
 PEAK.CURVECOEFFA
 PEAK. CURVECOEFFB
 PEAK. CURVECOEFFC
 PEAK. CURVECOEFFD
 PEAK.FITQUALITY

"Curve Type" can be one of the following {Average RF, Linear, Quadratic and Cubic}
 The coefficient values are set based on the curve equation described below:

Cubic : $A*x^3 + B*x^2 + C*x + D$
Quadratic: $A*x^2 + B*x + C$
Linear: $A*x + B$

If a value is not available then it will be 0. The values match those that are shown by OpenLAB ICM in its review calibration window.

Function: {AccessCode} ("R1","T1","P1; 3")

Run Type:

The run type for each record in the sequence table was not available for export. A new access code has been added to display this value. The RUNTYPE entry is accessible as follows:

Access Code: SEQUENCE.RUNTYPE

Instrument Control Updates

The Rapid Control (RC.NET) module has been upgraded to XXXXX version in this service pack release. This version adds support for new instrument control features and also includes some minor defect fixes.

5) Additional support for new and updated Instrument drivers

New Instruments supported:

- Agilent 1290 LC: Full Control

Updated Instruments drivers:

- Agilent 6890 GC: Updated Enhanced RC.Net driver update now supporting 7693A Autoinjector and Tray. Bar code reader is not supported by EZChrom.
- Agilent 6850 GC: New Enhanced RC.Net driver for the 6850, now supports full suit of inlets and detectors.
- Agilent 3000 microGC: New Enhanced RC.Net driver for the 3000 micro GC with the following general benefits:
 - Rugged RC.Net Architecture for better communication stability and driver portability.
 - Support of real time signal plot on screen for up to 4 channels.
 - Configuration diagram for each channel.
 - Localized user interface in Chinese and Japanese.
- Agilent 35900E ADC: The driver is now localized in Chinese and Japanese.

6) Automatic Method Migration from Classic LC Agilent methods

Automatic Method migration has been designed to facilitate method conversion from Classic Agilent LC to the enhanced LC methods. It assumes that no changes in the instrument configuration happened besides the driver type setting. If instrument hardware has change see the Method Resolution section below. Instrument drivers check for method consistency during the load operation. If a method is opened from a previous version of the driver, an automatic conversion attempts to convert all values from the previous method format to the current method format. When a method parameter is found to be missing in the new instrument driver, that parameter is dropped of the method with an entry on the system activity log and audit trail (upon method save). When a parameter in the new method cannot be mapped from the original method, a default value is assigned for it.

All sections of data analysis and reporting are moved along with the only risk being that changes in the detector signals break the mapping to the calibration. If signal channel assignments need to be changed, a new dialog box permits this change in the configuration screen for multi-detector configuration of Enhanced Agilent LC drivers. See "**Configuration of Detector Order**"

NOTE: Method Migration has been designed to be comprehensive, but a thorough review of the method is recommended. Documentation of method changes in the audit trail may be insufficient for compliance purposes.

7) Method Resolution

Enhanced Agilent GC and LC Instrument drivers (RC.Net driver types) check for method configuration consistency during the load operation. If a method setting is inconsistent with the current configuration the driver decides either to resolve without user intervention (i.e. automatic resolution, see above) or manually if user input is needed. In this version support was added to enable automatic method resolution. Please note that depending on differences in instrument configurations some parameters may not be migrated and may revert to default settings.

Loading an incompatible method into the method editor (instrument setup) that cannot be resolved will revert the method to the default settings.

Note:

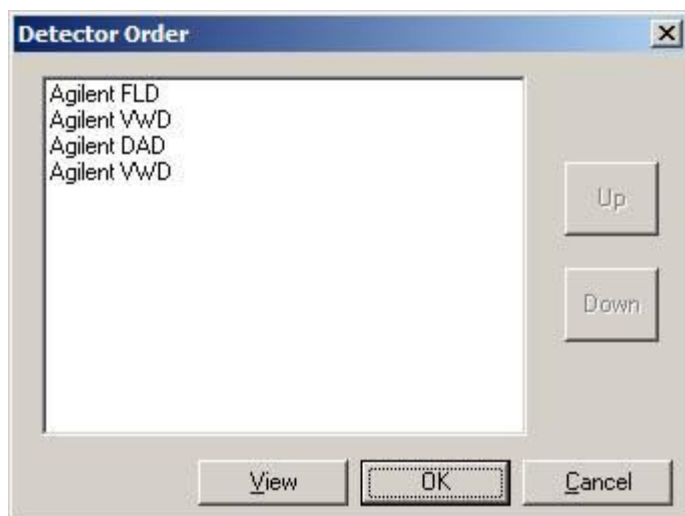
Incompatible methods used during sequence acquisition that cannot be resolved automatically will lead to the abort of the current run to avoid an invalid method running on the instrument. The sequence then proceeds with the next line in the sequence

This feature does not yet support resolution of Classic LC or GC driver methods.

8) Configuration of Detector Order

A new option is available within the instrument configuration for Agilent LC drivers to adjust the detector order when multiple detectors are present. It may be necessary to use this feature to match the detector order of a previously configured instrument when upgrading from classic drivers to the newer RC.Net driver or when configuring a new multi-detector LC that will use methods from another instrument. If the detector order between two different instrument configurations do not match, the signal options within the method (integration events, peak tables) may apply to the wrong signal.

To use this feature, select the button "Detector Order" in the instrument configuration dialog. This button will only be active for Agilent 1100/1200 instruments, and only when multiple detectors are added.



The detectors in the instrument configuration are shown. The View button can be used to view the detector order in the configuration. The Up and Down buttons can be used to adjust the detector order. Press OK and then save the instrument configuration to save these changes or select Cancel to discard the changes.

Other

9) EZChrom Elite Documentation is now copied to the installation folder

EZChrom Elite 3.3.2: Manuals are only available in the installation DVD.

EZChrom Elite 3.3.2 SP1: During installation a “Manuals” folder is created within the EZChrom Elite installation path, where related manuals and release documentation are copied. This applies to manuals provided by both the Service Pack 1 and the EZChrom Elite Add-on DVD 2.