

EZChrom Elite Compact

**What's New in
EZChrom Elite Compact 3.3.2
Service Pack 2**

Notices

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Agilent Technologies, Inc.
Stevens Creek Blvd.
Santa Clara, CA 95051 USA

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Using This Guide

Introduction

This Document lists the design changes introduced with Service Pack 2 for EZChrom Elite Compact 3.3.2. It describes new functionality that might differ from the previous behavior as described in the online help. Please note that the full version of EZChrom Elite had a Service Pack 1 but EZChrom Elite Compact did not have a Service Pack 1. Eventhough EZChrom Elite Compact did not have a Service Pack 1, features from Service Pack 1 in addition to features from Service Pack 2 have been rolled into EZChrom Elite Compact 3.3.2 SP2. These features are documented below.

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 In SP2

Data Analysis

1) Custom Parameter to support US Pharmacopeia Signal To Noise Calculation

EZChrom Elite Compact 3.3.2: EZChrom did not support the US Pharmacopeia custom parameter.

EZChrom Elite Compact 3.3.2 SP2: A new custom parameter has been added to support the US Pharmacopeia signal to noise calculation. This custom parameter does a signal to noise calculation according to the guidelines presented by the US Pharmacopeia. Once the custom parameter is turned on in a method, the reporting variables become available for reports and annotations.

Calculation:

The calculation used in the US Pharmacopeia is as follows:

$$S/N = 2h/h_n$$

h = The height of the peak corresponding to the component concerned

h_n = The difference between the largest and smallest noise values over a distance of 20 times the width at the half height of the peak.

The time range for the noise can be entered manually or automatically. If this value is to be calculated manually, the user must enter the first two parameters as start time of the noise and end time of the noise.

Using Custom Parameter:

To use the custom parameter add it to your method by browsing to Method → Advanced and clicking on the Custom Parameters Tab. Enter the following values:

Parameter Name – Enter any name (name should not contain a /)

Type – Enter Per-peak

Returns – Enter Number

Source – Click the blue arrow and browse to the C:\EZChrom Elite directory. Then, select the SignalNoiseUSP.dll file.

Additional Parameters: (These are optional parameters)

Parameter that will be used for actual calculation:

Start Time;StopTime – To manually enter the start and stop time for the noise. These parameters will be used in the US Pharmacopeia signal to noise calculation. If these manual parameters are not entered, the system will automatically use start and stop values from the calculation above.

Diagnostic parameters which give outputs:

;;NB – Outputs Noise Beginning (Start Time)

;;NE – Outputs Noise Ending (End Time)

;;VC - Outputs if calculation is good or bad (1 is good and 0 is bad)

;;NV – Outputs Noise Value – Calculated as (Max signal value – Min signal value) within noise time range

;;SV – Outputs Signal Value – Identical to Peak Height

****Note** – If this custom parameter was added after a run was acquired, you will need to perform an analysis before the parameter will show up.

The screen shot below gives examples of the additional parameters you can use. You only have to use 1 entry from the example below but you can use multiple ones.

Data Export		Graphics Export		Custom Parameters	Column / Performance	Files	Advanced Reports	
#		Parameter Name	Type	Returns	Source	Additional Parameters		
1	<input checked="" type="checkbox"/>	USP Signal To Noise	Per-peak	Number	C:\EZChrom Elite\SignalNoiseUSP.dll			
2	<input checked="" type="checkbox"/>	USP Start/Stop	Per-peak	Number	C:\EZChrom Elite\SignalNoiseUSP.dll	3,6		
3	<input checked="" type="checkbox"/>	USP Noise Beginning	Per-peak	Number	C:\EZChrom Elite\SignalNoiseUSP.dll	;NB		
4	<input checked="" type="checkbox"/>	USP Noise Ending	Per-peak	Number	C:\EZChrom Elite\SignalNoiseUSP.dll	;NE		
5	<input checked="" type="checkbox"/>	USP VC	Per-peak	Number	C:\EZChrom Elite\SignalNoiseUSP.dll	;VC		
6	<input checked="" type="checkbox"/>	USP Noise Value	Per-peak	Number	C:\EZChrom Elite\SignalNoiseUSP.dll	;NV		
7	<input checked="" type="checkbox"/>	USP Signal Value	Per-peak	Number	C:\EZChrom Elite\SignalNoiseUSP.dll	;SV		
8	<input checked="" type="checkbox"/>							

In the Column/Performance tab `“Calculate performance parameters for this channel” needs to be selected.

2) Signal Conversion Custom Parameter

EZChrom Elite Compact 3.3.2: The Signal Conversion custom parameter was not supported.
EZChrom Elite Compact 3.3.2 SP2: A new custom parameter has been added that allows you to calculate peak height and area using the actual signal numbers on the y-axis of the chromatogram without the use of multipliers. Once the custom parameter is turned on in a method, the reporting variables become available for reports and annotations.

Using Custom Parameter:

To use the custom parameter add it to your method by browsing to Method → Advanced and clicking on the Custom Parameters Tab. Enter the following values:

Parameter Name – Enter any name (name should not contain a /)

Type – Enter Per-peak

Returns – Enter Number

Source – Click the blue arrow and browse to the C:\EZChrom Elite directory. Then, select the SignalConversion.dll file.

Additional Parameters – Enter 1 for peak height and 2 for peak area

**Note – If this custom parameter was added after a run was acquired, you will need to perform an analysis before the parameter will show up.

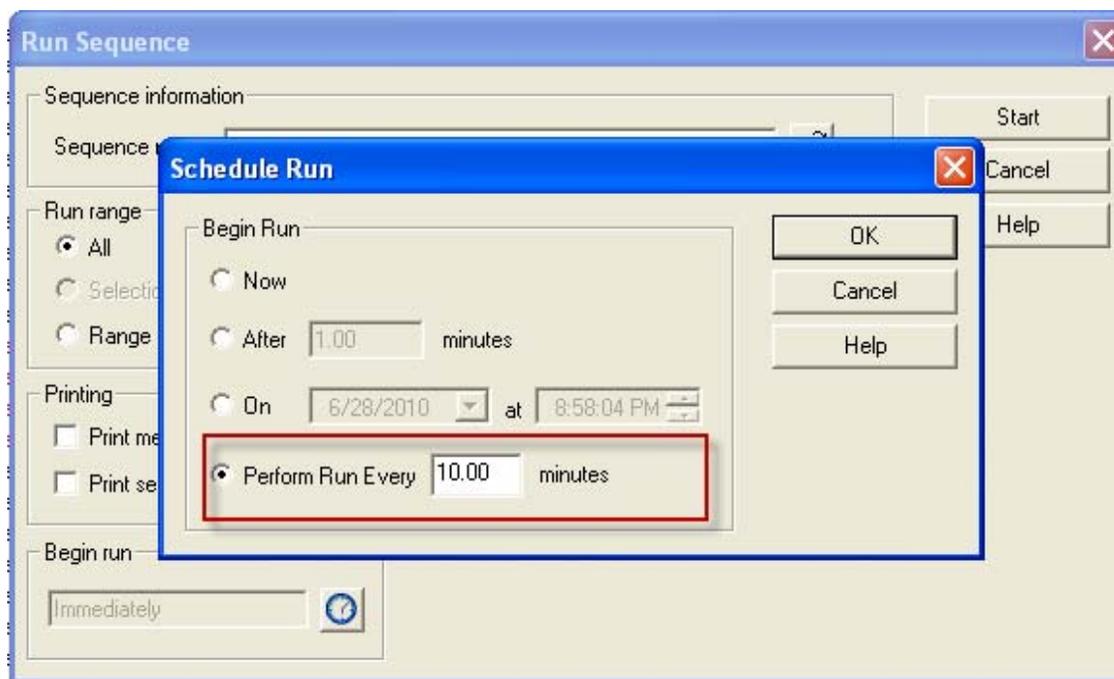
Data Export		Graphics Export		Custom Parameters	Column / Performance	Files	Advanced Reports	
#		Parameter Name	Type	Returns	Source	Additional Parameters		
1		Peak Height	Per-peak	Number	C:\EZChrom Elite\SignalConversion.dll	1		
2		Peak Area	Per-peak	Number	C:\EZChrom Elite\SignalConversion.dll	2		
3								
4								

Workflow Improvements

3) Perform Run Every X Min

EZChrom Elite Compact 3.3.2: You could schedule runs but you could not schedule a run at a specified interval.

EZChrom Elite Compact 3.3.2 SP2: The Perform Run Every X Min was added to allow you to schedule a run at a specified interval until the user aborts. When you use this feature an entry is added to the run queue at the interval specified and this continues until the user aborts their run. This can be accessed in the schedule run screen by clicking the clock under the Begin Run section. This is available for both single runs and running sequences. In the screen shot below an entry will be added to the run queue every 10 minutes until the user aborts.



Instrument Control Updates

4) Support for 1220 Compact LC Instrument

EZChrom Elite Compact 3.3.2: Does not support the new 1220 Compact LC.

EZChrom Elite Compact 3.3.2 SP2: This release of EZChrom will support the new 1220 Compact LC. Use the Agilent Compact LC driver when configuring a 1220 Compact LC (see below) and use AutoConfiguration to connect to the instrument. Please refer to the supported Modules and Firmware document for supported modules and firmware.

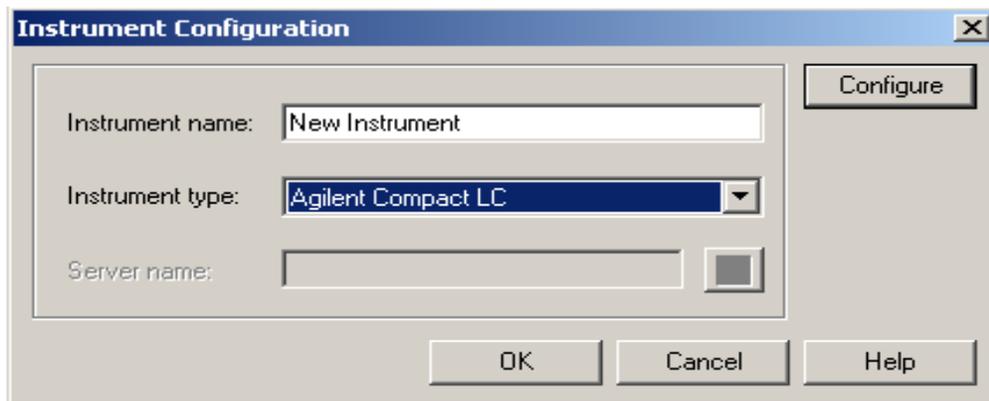
You will be able to configure 1100\1200\1260\1290 modules along with the 1220 Compact instrument. However, please note that a number of hardware configurations are limited due to functionality incongruity. Please contact support before adding an 1100\1200\1260\1290 module to a 1220 Compact to ensure compatibility.

5) LC Driver Name Changes

EZChrom Elite Compact 3.3.2: There was an Agilent Compact LC 1120 driver for configuring the Compact 1120 LC.

EZChrom Elite Compact 3.3.2 SP2: There is now an Agilent Compact LC driver for configuring both the 1120 Compact and 1220 Compact LC instruments. The Compact LC driver is localized in Simplified Chinese, Japanese, and Portuguese (Workstation only). When upgrading from a previous version of EZChrom all previously configured instruments will automatically be changed to the new driver. See screenshots below.

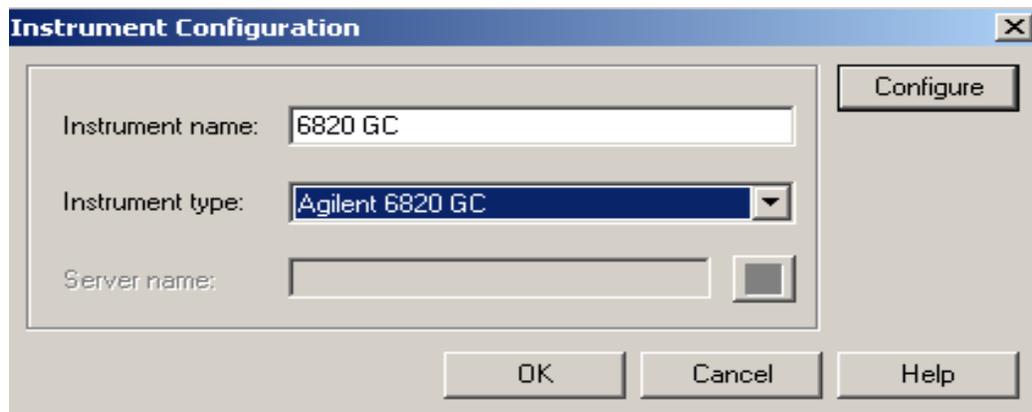
Use the Agilent Compact LC driver to connect to an 1120 or 1220 Compact LC



6) Support for 6820 GC

EZChrom Elite Compact 3.3.2: Does not support the 6820 GC instrument.

EZChrom Elite Compact 3.3.2 SP2: This release of EZChrom will support the 6820 GC. Use the Agilent 6820 GC driver when configuring an instrument (see below). The 6820 driver is localized only in Simplified Chinese. All injections are performed manually with this GC model. Please refer to the supported Modules and Firmware document for supported modules and firmware.



7) GC Driver Enhancements for 7820 GC

EZChrom Elite Compact 3.3.2:

- **Improved GC Method Resolution Behavior** - The 7820 would always attempt to perform method resolution when a method did not match the instrument configuration. This could prevent reprocessing of existing data if the instrument had been reconfigured since the original data was acquired.
- **GC Column and ALS Configurations Controlled by Method** – The 7820 maintained all GC configuration data in the instrument configuration, including parameters that may be changed by end users. As a result, instrument operators needed roles that allow instrument configuration in order to execute typical GC workflows like changing columns or injector syringe sizes.

EZChrom Elite Compact 3.3.2 SP2:

- **Improved GC Method Resolution Behavior** - EZChrom does not invoke GC method resolution when reprocessing existing data in an offline session. An additional enhancement is the movement of several user-configurable instrument options from the instrument configuration to the method. Method resolution therefore will only occur if the physical GC or ALS hardware has changed.
- **GC Column and ALS Configurations Controlled by Method** – The new GC drivers now store ALS parameters and GC column information in the method and not in the instrument configuration. These parameters can be found and edited in the **Configuration** tab of the GC instrument method. With these changes, more control is given to the instrument operators without the need to enter instrument configuration. However, these changes also require the operators to take more care to ensure that methods are compatible with the instruments they are run on.

Impact On Instrument Configuration

- Physical instrument information such as inlet and detector types, valves, Aux options, connected ALS modules and ALS tower positions are still stored in instrument configuration.
- If any changes are made to these physical parameters of the instrument, the instrument must be reconfigured in EZChrom, and the most current configuration uploaded from the GC.
- No physical instrument parameters can be edited in the EZChrom configuration dialog; they can only be read from the GC.

Impact On EZChrom Methods and Workflows

- When porting a method from one instrument to another, if the instrument configuration (hardware) does not match the method configuration, then method resolution is invoked to make the method compatible with the hardware as recorded in the instrument configuration. This may occur when a method is used on two different instruments with different ALS models or options.
- Since the GC column information is now stored in the method, it is necessary for the operator to ensure that the instrument itself has the appropriate column(s) installed as indicated in the GC method's column configuration section. If this is not done, then the instrument may attempt to set pressures and flows that cannot be achieved; resulting in errors or module shutdown events.

- When ALS parameters now stored in the method, it is necessary for the operator to ensure that the physical instrument matches the settings in the method. For example, the operator must verify that the syringe size designated in the method is actually installed in the ALS injector. Otherwise the actual volume injected may be incorrect or the ALS may raise an error indicating an invalid injection volume.
- The same care must be taken when porting sequences from one instrument to another. The sequence control depends on the ALS options and injector tower positions. For example: a sequence created for dual-tower operation will fail with an error when run on a GC with only one injector tower configured.

List of Items From SP1 Rolled Into SP2

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

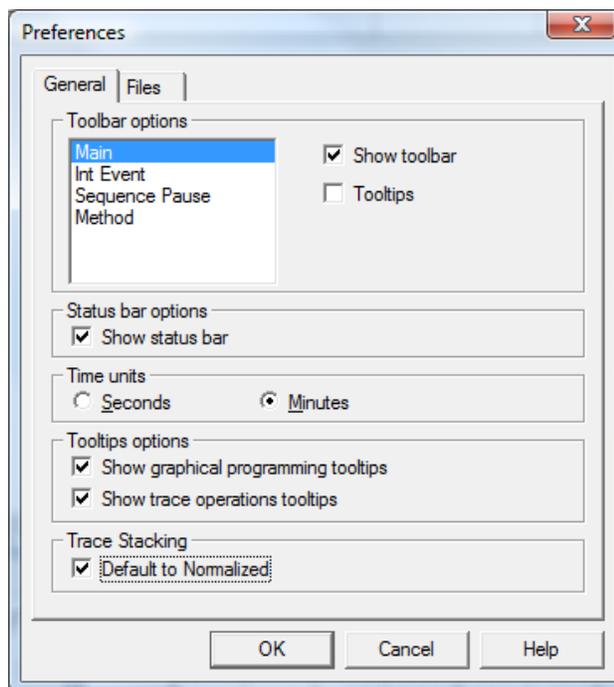
Signal-to-Noise Ratio

EZChrom Elite 3.3.2 SP1: New custom parameters has 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

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