# Software Update Notification



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Product	PartNoIssue
Software suite	PSS0012-10

Product	PartNo./Version
Zetasizer Nano series	PSW0085/4.10
Firmware	PFW0044/1.31

Manuals	PartNo./Version
Zetasizer Nano series	MAN0317/2.20
MPT-2	MAN0318/2.10
HPPS	MAN0314/2.00

# Software update summary

Main features
Addition of selection of units for a number of parameters, e.g. Radius/diameter
Addition of a statistics bar to the records view.
The method for adjusting the pH during a pH titration has been simplified and the time required reduced
A single button implementation of a fast mode for the correlator settings has been added to the research software
Addition of ability to do CMC titrations
Addition of facility to monitor sample count rate without starting measurement
Addition of a new analysis type to the research software - Discrete Exponential Analysis
All parameters are now displayed to a defined format

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## 1. Overview

This document is the software release note for Zetasizer Nano series software P/N PSW0085 on software suite PSS0012-10 in accordance with DCO4113

## 1.1 Main feature comments

## 1.1.1 Unit selection

It is now possible to select the units for a number of parameters. The data in a record is stored in a pre-defined format that cannot be altered. The units that are actually displayed are defined by the user workspace. This means that a particular record can be displayed in different formats depending on the workspace settings of the particular user displaying the data.

The units are linked in all places that they are displayed. This means that the units will always be consistent in a particular workspace setting.

The heading in the record view now consists of two lines, the top line being the parameter name, and the second being the parameter unit. Where there is an option to change a unit, left or right clicking on the unit will give a selection of the units available. Clicking on a unit will change the unit name on the second bar, and also change the numerical value of the unit displayed in all the records being viewed.

Simultaneously, all references to this parameter will change in the reports selected, and in the SOP settings.

The parameter units can also be changed within a report by right clicking on a unit, or in an SOP page, and similarly this will change all occurrences of the display of the parameter. These unit settings will be stored with the workspace.

## 1.1.2 Statistics bar

A statistics bar has been added to the bottom of the record view. This can display a maximum of four parameters, mean, standard deviation and maximum and minimum values. Selection of the bars to view is either by right clicking on any displayed bar, then selecting 'Statistics bar and the parameter required, or by selecting the 'statistics bar' option from the 'View' menu. The bar will display a value for all numerical parameters for the records selected. Records are selected in the normal Windows fashion using click and drag, or combinations with the shift and control keys.

The record numbers for the records selected are displayed in the top bar that is displayed. A range of records is displayed separated by a bar, e.g. 1-7, and non-contiguous records are separates by commas. A combination of these methods is also used, e.g. 1-7,15, 23

## 1.1.3 Titration algorithm

A new method is implemented for pH autotitrations. This new method will shorten the time taken for a titration without having to use a pre-scan. It takes sample buffering into account and is designed to avoid overshooting the target pH. Back titration is not allowed, and this avoids any tendency to 'hunt' for the correct pH value, which could previously add to the measurement duration.

The success of the titration, i.e. reaching each of the target pH values in a reasonable time, without overshooting still relies on a well calibrated pH probe in good condition.

The ability to measure a buffer correctly, and stabilise in a short time is not a good enough test as this does not duplicate the performance of the probe in a real sample.

After calibration, a better test is to measure the pH of a known concentration of a strong acid or base. For example a 1 millimolar solution of Hydrochloric acid should be pH 3. In such a test the pH measured should be within 0.1pH units of the expected value.

Note that SOP's originally set up in version 4.00 that used a pre-scan, will still enable the prescan method to be used, however SOP's created using 4.10 will not allow this method. There is an option to retain the pre-scan method if required, please contact Malvern Instruments UK for details.

#### 1.1.4 Fast correlator mode

The method of implementing the fast mode of the correlator available in the research software, has been simplified. There is now a single radio button to enable or disable the fast mode. It is disabled as default, as this is the default setting in the standard software. Enabling the fast mode adds 16 channels of 25ns each, starting at 25ns. As the response time of the detector does not allow pulses to be generated at intervals of less than 50 ns the first channel displayed is at 75 ns. In addition, the logarithmic correlator, which as default has the first channel at a delay time of 0.5 microseconds, will start at 0.25 microseconds. Note that if the fast mode is implemented, even though the analysis may use the same delay times as the default settings, there can be subtle differences in the result due to the different integration times used by channels with the same time value.

#### 1.1.5 CMC titrations and poor data

Whenever multiple measurements are done, it is now possible for the measurement to continue even though the data collected cannot be analysed.

In the case of a titration, error suppression is automatic. In this case, an error message with a timer will be displayed. If a user does not interrupt the measurement, the correlation function will be stored, and the measurement will continue at the end of the timed period.

This is useful in the case of a concentration titration, for example, to determine the critical micelle concentration (CMC). Below the concentration that micelles appear, the data may be too poor to analyse, but the intensity information could still be useful, and the data is likely to improve at higher sample concentrations.

In the case of a temperature trend measurement, or a time trend measurement done by specifying a number of repeat measurements, the error message can be suppressed by selecting, 'allow results to be saved containing correlation data only'.

## 1.1.6 Sample count rate monitor

A count rate meter is available that shows a continuous display of the sample count rate without having to start a measurement. The option is available under the 'Tools' menu. A dialog box displays the count rate and gives the user has access to the attenuator settings and the cell type used.

Selecting the cell type displays the default measurement position for that cell. The user can accept this by selecting the 'set' button.

In a similar manner, the user can change the attenuator setting by selecting the attenuator required, then selecting the 'set' button to change the attenuator to that setting.

If a measurement is started, this dialog box will close and the Tools menu item will be greyed out.

## 1.1.7 Discrete Exponential Analysis

This is an addition to the research software, designed particularly for protein samples. This analysis allows the user to input information known about the sample to give more precise information about the proportion of up to three components in the sample. There are two method of inputting information. The sizes of expected components can be chosen, or alternatively the number of multimers of the second and third peak can be specified.

The result gives the size and proportion of the two or three peaks detected. No peak width is calculated as it is assumed in this special case that each peak consists of a single size component.

More advice is available in the sizes tab after the Discrete Exponential analysis has been chosen.

#### 1.1.8 Parameter format

All displayed parameters now have a defined format. The parameter will be defined either as text, with properties such as the maximum length allowed, or numeric, with a definition of the format such as exact display, e.g. correlator channel contents, or a defined number of decimal points, e.g. 1 for the temperature.

For simplicity all parameters are assigned to categories which then have the same format properties. 'Size' is one class of format and in this case, the display is to 3 significant figures. This format to a number of significant figures has not been available before, examples in the case of the size class are; 0.678nm, 1.23nm, 12.3nm, 123nm, 1230nm.

## 2. Compatibility

## 2.1 Optics unit

Version 4.10 software is compatible with all hardware variants of the Zetasizer Nano series and the HPPS.

## 2.2 Data

Version 4.10 will read data from all versions from 3.xx and 4.00. It will not read data from Version 1.00 or V1.10 software. If data taken with a previous version is edited, even if only the sample name is changed, the result can change due to small changes designed to improve the analysis.

## 2.3 Computer

#### 2.3.1 Operating system

Version 4.10 is only compatible with Windows 2000 Pro (Sp4 or later) and Windows XP Pro (Sp1a or later)

Windows XP Pro is the preferred option as the complete alpha test has been performed on this operating system.

NOTE: Windows NT and Windows XP 'Home' version are not supported

## 2.3.2 Minimum Computer Requirements

Pentium PC 233MHz, 128MByte RAM, 20MByte free hard disk space, 1024 x 768 screen resolution, CD-ROM drive, 1 free USB port, Windows 2000 Pro (SP4 or higher) or Windows XP Pro (SP1a or later) operating system.

Use with the HPPS requires one free PCI slot

The software and system can be used with a laptop computer with a free USB port. Use of a laptop with the HPPS requires a free type 2 PCMCIA slot and a special PCMCIA card. Please contact Malvern Helpdesk for details. The PC must meet the minimum requirements of the operating system software.

The PC must meet the minimum requirements of the operating system software.

## 2.3.3 Recommended Computer Requirements

Pentium P4 PC 2.6GHz, 512MByte RAM, 40GByte hard disk drive, 1024 x 768 screen resolution, CD-ROM drive, USB port, Windows XP Pro (SP1a or later) operating system.

The software and system can be used with a laptop computer with a free USB port. Use of a laptop with the HPPS requires a free type 2 PCMCIA slot and a special PCMCIA card. Please contact Malvern Helpdesk for details.

# 3. Functional Features, changes since version 3.32

## 3.1 Additions

SCR	Description
2553	Addition of facility to monitor sample count rate without starting measurement
2940	Option to reset temperature to ambient after temperature trend measurement
4232	Option to append measurement number to sample name after zeta potential and size trend SOPs.
4292	Correlogram will now be saved even if data cannot be analysed
4234	The measurement can be initiated immediately by selecting the start icon. The measurement will then start after temperature equilibration is complete.
4352	The trend table properties can be configured from the main application as well as from the from the report designer.
4365	An option is added to reset the temperature to a defined value at end of a temperature scan
4372	Addition of a new analysis type to the research software - Discrete Exponential Analysis
4391	Addition of ability to edit many results simultaneously
4410	Addition of titration tutorial for the MPT-2
4460	Addition of pH read back during an additive titration
4466	Addition of % over/under plots to the zeta potential statistics graph
4479	Addition of ability to do CMC titrations
4484	Audible indication on completion of SOP
4606	Addition of normalised diffusion output from White-Mangelsdorf calculation
4658	Addition of reference beam count rate, measured voltage and measured current parameters to recorded data
4665	Addition of second virial coefficient error and correlation coefficient parameters
4671	Addition of selection of units for parameters
4673	Addition of a statistics bar to the records view.
2869	Reference beam count rate should be available as parameter in zeta measurement records.

## 3.2 Deletions

None

## 3.3 Changes

SCR	Description
4440	The method for adjusting the pH during a pH titration has been simplified and the time required reduced
4489	The Integration method for the White-Mangelsdorf calculation has improved accuracy
4508	Sub-runs can be saved for zeta potential measurements in the research software
4631	The reports have been changed to take alteration of parameters and display of units into account
4648	A single button implementation of a fast mode for the correlator settings has been added to the research software
4652	Parent and child records are now always shown even if one of the record types doesn't match the workspace settings.
4672	All parameters are now displayed in a new defined format
4709	The stirrer in the MPT2 is now activated when the "pH Monitor" tab is accessed

4730	MPT2 tutorials have been updated.
4779	Molecular weight: Count rates for the scattering standard and the solvent are
	now displayed before the operator is prompted to accept them.
4760	MPT2 pre-measurement clean and prime message prompt has been updated.

## 3.4 Bug Fixes

SCR	Description
4178	The tab key now sets the focus to material or dispersant properties tabs on the sample page.
4490	The selection of cutoff/number of points in research software (Edit Result) is corrected
4547	The create average result feature error when averaging zeta results generated using the monomodal analysis type is corrected
4557	Titration measurements would fail under Windows XP unless running with Administrator privileges.
4603	The cell position is reported correctly as 2.00mm for zeta measurements taken on a 90 degree size measurement system.
4641	The default size analysis settings have been corrected
4647	The number of analysis points are now correctly set
4651	Errors in the cumulants analysis for the HPPS have been corrected
4653	The Alpha value is now stored correctly
4655	The cumulants settings for the OQ SOPs supplied have been corrected
4657	The size limits displayed are now correct in the OQ SOPs
4660	The correlator page has an interim fix for the parameter settings
4662	Errors in coated sphere model have been corrected
4677	Problems with Runge Kutta solver in White Mangelsdorf calculation have been corrected
4684	The parameter dictionary text name for the distribution analysis threshold (lower and upper) are now correct
4710	Checking the "Enable Stirrer" box in the "Clean" and "Fill" tabs now activates the stirrer
4734	Removed molecular weight measurement type from SOP editor for 90° instruments.
4743	Molecular weight fit error is now reported correctly.
4772	Derived mean count rate, i.e. without the reference beam, is now stored correctly during zeta measurements.
4781	Temperature is no longer set to 25°C when measurement window is closed.

## 3.5 Known Issues and comments

## 3.5.1 USB Detection

USB detection occurs automatically on new computers. On older computers the instrument is not always detected automatically and the instrument icon in the bottom right-hand corner of the status bar will remain greyed-out. This is fixed by closing the application, restarting the computer and restarting the software.

#### 3.5.2 Missing parameters in user reports

The parameter dictionary has been updated for this version of the software and some of the parameters have changed. For reports that the user may have created containing the affected parameters, the parameters will become undefined. This can be seen when a report is opened and the parameter displays the text 'No parameter has been selected' or nothing is shown next to the text label (i.e. the value appears blank). To fix this problem for each parameter carry out the following steps:-

- 1) Double-click on the affected parameter to bring up its property dialogue.
- 2) Click the 'Select' button to display the 'Select a parameter' dialogue.
- 3) Select the relevant parameter.

**N.B.** Remember to correct the affected parameters on both the screen and page layout views of the report.

## 3.5.3 Results

The analysis algorithms for the calculation of size, zeta potential and molecular weight, including data filtering, are being continually improved. The effect of this is that if data taken from a previous version of software is edited, the result may change, even if only the sample name is edited.

This is because the algorithms themselves are not stored with the record.

This does not apply to parameters stored with the record such as the viscosity, and refractive index etc. as the same parameters are always used in the recalculation of the edited result.

This does not of course change the result in the stored record, as after editing a new record is created. To tell if a record is the original or has been edited, the parameter 'Is edited' can be added to a report or the record view. This can be found in the measurement audit information section of the parameters list. It will display 'False' if the record has not been edited.

#### 3.5.4 Manual measurement settings

Installing version 4.10 software will cause the manual measurements settings to revert to their default values. After installation any changes are preserved between settings.

# 3.5.5 Application error when editing the analysis limits of existing zeta measurement records

Editing the zeta potential range of an existing record may cause an error, and the software will have to be shut down. This editing is mostly required when measuring samples in low dielectric constant media, or when using very low voltages.

A suitable range should be set before the measurement. For a sample in a dispersant with a very low dielectric constant such as hexane, the zeta potential range in the results calculation page, under the advanced button should be set to -500mV to 500mV

#### 3.5.6 Latest firmware required when running SOPs created with version 4.10 software

This is a problem for existing users if an SOP is created with version 4.10 software without having the instrument connected on start-up (so the firmware is not updated). If the instrument is then connected (without restarting the application) and an attempt made to run the SOP then it will fail with the error message shown below:-

DTS	
8	This SOP has been designed for a different instrument type or instrument configuration.
	run the SOP again.
	СССК

The fix for this problem is to restart the application with the instrument connected.

#### 3.5.7 The following SCRs detail issues that currently exist within the software.

SCR	Description
2364	Export Data dialog does not remember the last destination filename and path that was used.
2650	Unexpected filling using the Filled Graph option
2653	Can set the warning and action limits wrong way round
2657	Melting point SOP dialogs should display a warning with fixed temperature dispersant
2735	Dragging records onto desktop fails
2746	Tables have insufficient numerical precision
2855	Clicking on a measurement or report file from the "Start->Documents" toolbar fails to open
2881	It should not be possible to delete a security group if there are users in it.
2882	Deleting a group should be audited
2883	It is currently possible to add a user without specifying any group.
3005	Melting Point - automatic run duration may not be suitable choice
3066	Graphs - The statistics graph does not correctly support the Weight transformation
3130	No warning message when running a zeta, molecular weight or melting point SOP on a HPPS.
3131	User reports will not print unless they are added to the current workspace.
3151	Zooming in on a graph does not refresh the tick labels.
3186	21 CFR - Can create a group with the same name as an existing group.
3411	Dielectric constant value should change with temperature.
3491	If the software can not access the registry it gives a run-time error
3714	Record browsing in print preview does not work
4067	User ->New User menu does not force values in password and password confirmation boxes.
4123	Not possible to change the name of a Workspace
4143	Protein Utilities: Pasting a graph into Wordpad changes the graticle line style
4169	Audit trail does not record the copying of records
4237	Research Software:Edit Result, no explanation on coated sphere
4286	Number of runs still tries to limit the measurement to 6 hours, instead of allowing 10,800
4345	Record appears selected when it isn't
4405	Add ability to use own larger beaker
4407	Allow increment and points option in dilution titration
4414	Zeta edit result not possible for monomodal measurement data

#### Zetasizer Nano series Application Software for use with (English) Microsoft Windows 2000 Pro and Windows XP Pro

SCR	Description
4427	Problems with default printer can cause the application to crash
4446	Printing the record view exhibits different behaviour than printing a report
4488	Cannot batch print to pdf
4539	Size measurement optimisation routine should follow temp equilibration
4553	Add temperature coefficients
4610	Current Record selection is deselected if a new report is added
4616	Cannot view a read-only audit trail file.
4617	Software freezes when attempting to open a none audit trail file in the audit trail viewer

# 4. Installation

## 4.1 Installation Procedure for Windows 2000 Pro

# You must uninstall the previous version before installing the new version. See the 'Uninstall procedure' below.

The software suite comes on an auto-loading CD-ROM. Inserting the drive into a system configured to Auto-run a CD will run the installation program automatically. If your system does not support this feature run the **\setup.exe** program from the root directory of your CD drive.

## 4.1.1 Record view headings

The new record view unit headings will not be displayed unless the existing workspaces are deleted. The current headings are stored in a file automatically named as the user currently logged on to the computer with a '.wrkspace extension'. e.g. JOHN SMITH.wrkspace To access the new headings this file must be deleted or renamed after the uninstallation procedure.

After uninstalling the software navigate to the 'C:\Program Files\Malvern Instruments\DTS' directory. This will contain the user workspace. This can either be deleted, in which case a new user workspace will automatically be created during the installation process, or it can be renamed to allow its use later. Note only the '.wrkspace' extension can be used. During the installation a new workspace will automatically be created, and the new record headings will then be displayed.

## 4.1.2 Example data

The examples data file has been updated.

To access the new examples file the old file must be deleted or renamed after the uninstallation procedure and before the new software version is installed.

After uninstalling the software navigate to the 'C:\Program Files\Malvern

Instruments\DTS\Measurement Data' directory. This will contain the example results.dts file. This can either be deleted, or it can be renamed to allow its use later. Note the '.dts' extension must be used to enable access to a file from within the application. During the installation the new example results will be installed.

The example data is most conveniently viewed in the summary workspace as all the reports to view the data are available in this workspace.

**Note:** If the system has a previous version of 3.xx or 4.xx installed, then this must be uninstalled before version 4.10 is installed as it cannot be co-resident. Version 1.10 (HPPS) can be left on the system and version 4.10 installed

**Note:** On the instrument selection screen, the type of instrument, laser wavelength and scattering angle must be specified. Text information is supplied on this screen to help with your selections.

**Note:** For DTS Series software, Windows 2000 <sup>™</sup> Pro and Windows XP <sup>™</sup> Pro will not allow an installation if the user does not have administrator access. This is in line with Microsoft's Logo policy and is standard practice.

**Note:** Windows 2000<sup>™</sup> Pro systems require service pack 4 or later in order to install the software.

## 4.2 Installation Procedure for Windows XP Pro

Windows XP may give the following warning during the installation. This warning can safely be ignored by clicking 'Continue anyway' as the software installation has been tested on Windows XP.

Software Installation	
1	The software you are installing has not passed Windows Logo testing to verify its compatibility with Windows XP. (Tell me why this testing is important.)
	Continuing your installation of this software may impair or destabilize the correct operation of your system either immediately or in the future. Microsoft strongly recommends that you stop this installation now and contact the software vendor for software that has passed Windows Logo testing.
	Continue Anyway

## 4.3 USB Driver Installation

**Note:** Driver installation on Windows 2000  $^{\text{TM}}$  Pro and Windows XP  $^{\text{TM}}$  Pro will fail if the user does not have administrator access. This is in line with Microsoft's Logo policy and is standard practice.

## 4.3.1 Windows 2000

With the software installed the instrument should be connected via the USB port. The drivers should now be installed automatically without any user input.

#### 4.3.2 Windows XP Pro

With the software installed the instrument should be connected via the USB port. This will result in the found new hardware dialogue appearing:



This should be left with the default selection of 'Install the software automatically' and the 'Next' button should be pressed so that file transfer begins. During file transfer a similar warning dialogue as appeared in section 6.2 may be displayed. Once again the 'Continue Anyway' button should be pressed so that file transfer completes. Once file transfer has completed the 'Finish' button should be pressed to complete the installation.

## 4.4 Uninstall Procedure

The software can be uninstalled using the standard Add/Remove feature in the Windows 'Control panel'

## 5. Customer deliverables

## 5.1 Application Software Suite

The software is contained on one CD-ROM. The disk is labelled PSS0012/10 The installed software requires about 80Mbytes of hard disk space.

#### 5.1.1 Disk contents

- Operating software including update help files for all new features plus tutorials
- Zetasizer Nano series operators guide, Issue 2.20
- MPT-2 Operators guide, version 2.10
- HPPS Operators guide, Version 2.0 (Covers up to version 3.00 software. Later features are covered in the help files)
- Firmware version 1.31
- USB drivers for the Zetasizer Nano
- Hardware drivers for the HPPS, for both desktop and laptop operation
- Software Update Notifications for all versions of software from version 3.00 to present
- Adobe Acrobat reader