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Technical Services and Scientific Equipment

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# Creoptix WAVE (Malvern)

## Short Usage Notes

➢ **Before to start**:

- The use of the instrument is permitted **only after having obtained a specific training**. Contact the Facility Staff for more information.
- This document does not replace the manuals. The user is invited to look carefully at the manuals (hardware and software) available in the facility website.
- The instrument should be used only for its intended usage. Any other usage is forbidden. In particular, **it is strictly forbidden to alter in any way the instrumentation** (e.g. by removing or adding components, etc.).
- It is forbidden to install any software, unless authorised by the Staff.
- **Do not move or displace the instrument.**
- **The instrument should NEVER be let dry or without any flow. At the end of the session the User should replace the buffer with milliQ water, insert the Maintenance chip, and leave the instrument in Standby Mode**.
- **At the end of the session the User MUST remove all the samples used and dispose on their own of the waste**.
- **NEVER operate the instrument without a chip**. **A chip must always be inserted**.
- All buffers used must be filtered and degassed.
- In case of doubts and for any issues **always contact the Staff** before taking any initiative.
- The instrument is accessible with the **Single Sign On system (SSO)**.
- The use of any external device (e.g. USB-key) is not allowed. Use the Drive to transfer data.

➢ **Turning on.**

- Turn on the computer.
- Launch the WAVEcontrol software
- Turn on the WAVEsampler, then the WAVEcore (buttons on the rear, see Figure 1).
- In the Device tab, the device will appear once connected

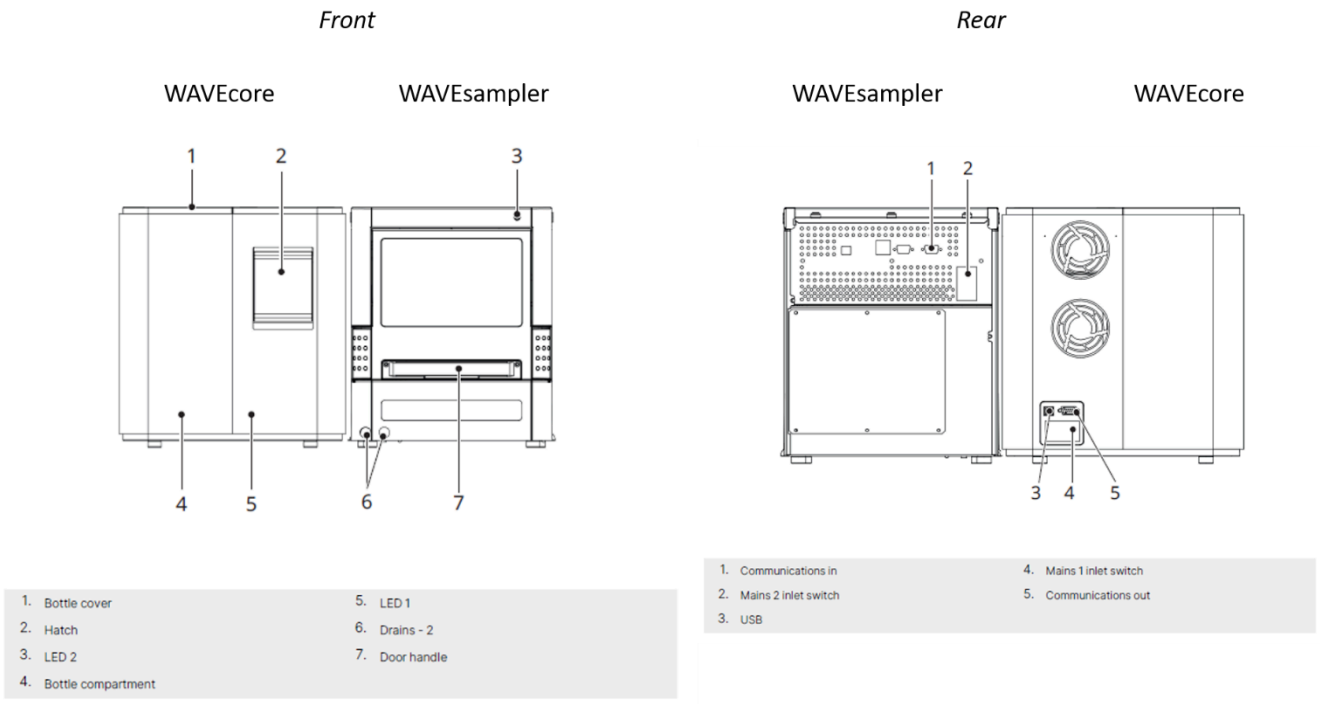


*Figure 1.Front and rear of the instrument. ON/OFF marked by numbers 2 and 4 (rear).*

## ➢ Operation with WAVEcontrol.

- The main window of the WAVEcontrol program looks like in Figure 2.

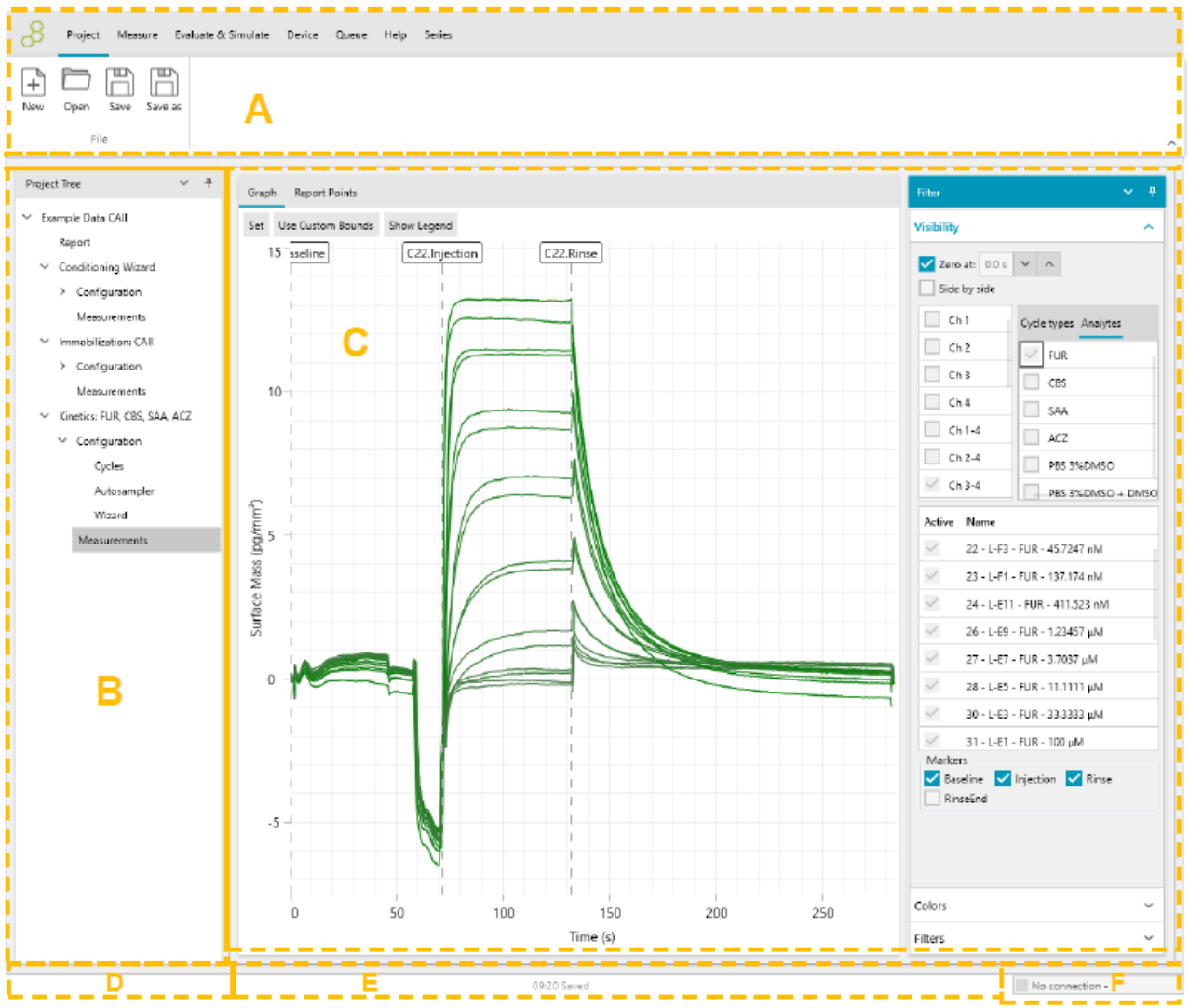


*Figure 2. Main window. A. Main Menu. The main menu is divided into the following subsections: 1. File 2. Measure 3. Evaluate & Simulate 4. Device 5. Queue 6. Help B. Project tree. Organizes all data of the experiment for a one-click access. C. Main Panel. Depending on the navigation within the main menu and project tree, contains the configuration, measurement and evaluation views. D. Queue status bar. Contains queue runtime information. E. Project status bar. Notifies about file status. F. Device status bar. Notifies about device status.*

- The main window is divided into different parts with different functions (Figure 2).

  A. **Main Menu**. The main menu is divided into the following subsections:

  1. File 2. Measure 3. Evaluate & Simulate 4. 5. Queue 6. Help

  B. **Project tree**. Organizes all data of the experiment for a one-click access.

  C. **Main Panel**. Depending on the navigation within the main menu and project tree, contains the configuration, measurement and evaluation views.

  D. **Queue status bar**. Contains queue runtime information.

  E. **Project status bar**. Notifies about file status.

F. **Device status bar**. Notifies about device status.

## ➢ Getting started

- Prepare buffer and waste bottles
  - Prepare **fresh, filtered and degassed** buffer in an appropriate bottle and connect to the buffer pump (Figure 3). (*As a rule of thumb, ca 200 mL of buffer are needed for the initial setup, and ca 300 mL to run a 7 points kinetics with 2 replicates. 25 mL per day are needed for Standby mode*).
  - Make sure that the waste bottle is empty and connected to all the four waste tubes (Figure 3).

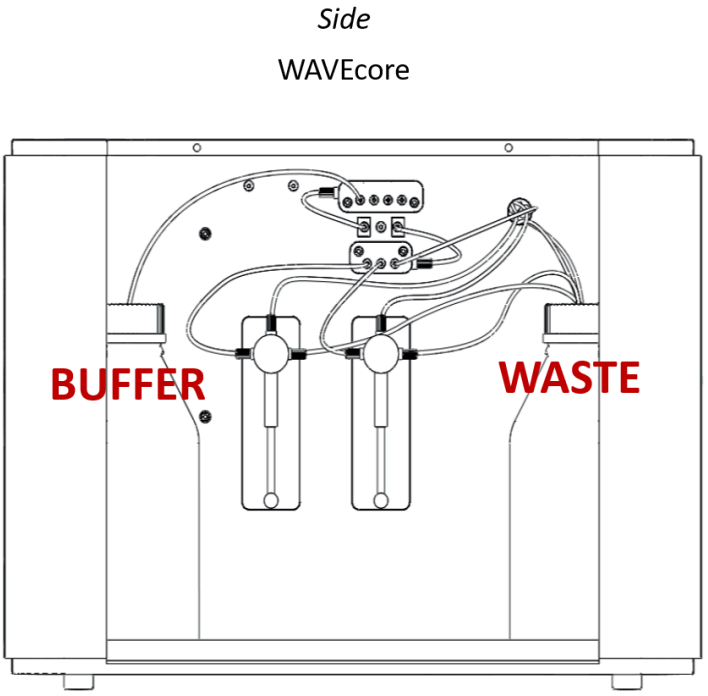


*Figure 3. Buffer and waste bottles.*

- Create a new project (Project>New). Save the project (Project>Save As). Once the project is created, new data are automatically saved during the experiment.
- At the beginning of the session, execute at least one initial prime if the instrument was in standby (Device>Initial Prime). This will prime the pumps. This is not needed in case you change the buffer (see the corresponding instructions)
- Execute at least one chip prime (Device>Chip Prime). This is not needed if you insert a new chip or if you change the buffer (in that case follow the corresponding instructions).
- Execute at least one buffer exchange (Device>Buffer Exchange) if you have connected a new buffer. This operation consumes ca 25 mL of buffer and corresponds to 3x Initial Primes and 3 x Chip Primes. This step can be omitted if the buffer is not changed. This step should be always performed after the buffer changes. **NEVER change directly from an organic solvent to an aqueous buffer, and vice versa: this would cause precipitation and block the system.**

**ALWAYS interleave a step with pure water (milliQ). This is necessary also in the case of incompatibility among components of two different buffers**.

- Insert a chip:
  - Open the hatch (Figure 4).
  - While keeping the cover open with one hand, gently insert the chip like indicated in Figure 4 (fluidic on the upper part), until it stops.
  - Close the hatch.
  - Select the correct option from the automatic prompt window (New Chip and New Buffer, New Chip, Maintenance Chip). The system will automatically perform a buffer exchange, if the case, and a chip align.

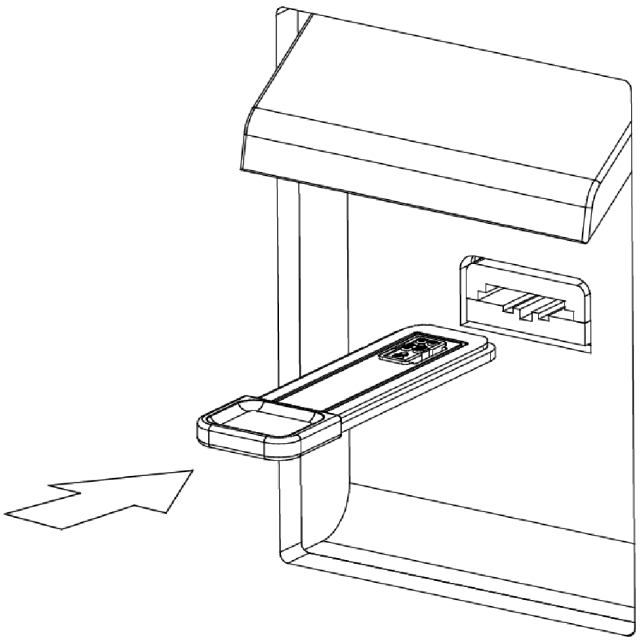

*Figure 4. Insertion of the chip.*

- Align the chip, if you didn't insert a new chip (Device>Chip Align).
- Check the amplitudes (Device>Live View). **The amplitudes for all the flow cells must be larger than 50**. If it is not the case, perform a chip align and/or a chip prime again. Note that if the amplitudes change considerably (±10%) it might be a sign of the presence of air in the chip. In that case prime and align the chip again until the amplitudes are stable.
- Prepare the autosampler:
  - Open the WAVEsampler
  - Insert the tube rack and/or 96-well plates (Figure 5)
  - The sample position and info in the sampler are defined and edited in the Autosampler menu once a wizard is created (Figure 5).
  - **IMPORTANT: always consider a dead volume of 20 µL for conical shaped vials/wells and of 400 µL for flat bottom vials. Whenever the system provides volumes to be prepared, always ADD the dead volume to the required volume.**

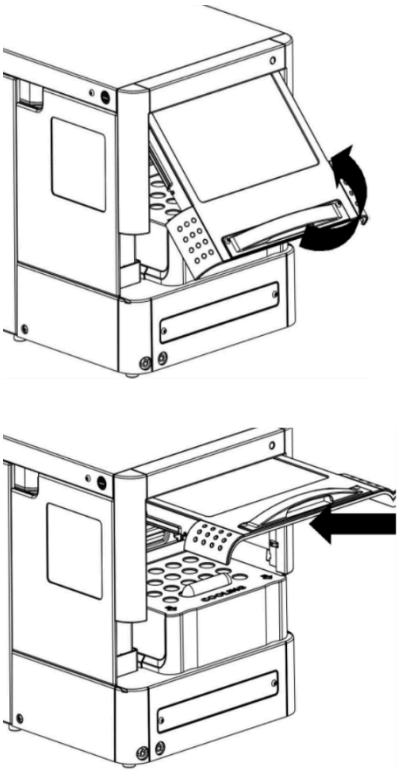


*Figure 5. Autosampler opening (left) and panel (right).*

## ➢ Setting up and running a measurement

- Each measurement is very different as it is sample dependent, therefore only general guidelines are provided here. The precise strategy and flow path have to be identified by the User. The Staff is there to help.
- A series of wizards to run the different steps of a project is available under Measure. It also possible to run manually a method (see the Manuals for that)
- The following wizards exist:
  - *Conditioning*: Use this wizard for chip conditioning. Simply select which chip type, and optionally which buffer you are using.
  - *pH scouting*: Use this wizard for testing optimal immobilization conditions for amine coupling. Simply add your Ligands and corresponding pH conditions, and regenerations you wish to test, to the corresponding lists, and click “Create Series”. It is recommended to move from milder to harsher conditions.
  - *Immobilization*: Use this wizard for ligand.
  - *Kinetics*: Sets up the series for a kinetic interaction where the software optimizes the plate layout.
  - *Regeneration-Free Kinetics*: Use this wizard for measuring a tight interaction without regeneration.

- *Screen*: Use this wizard for setting up a screen where the plate layout is given, as described in below section Screen wizard

○ To run a wizard, select the desired the wizard and follow the instructions, inserting the pertinent information. Click on create series. Once the series are created, hit Series>Run in order to run a method (Figure 6).

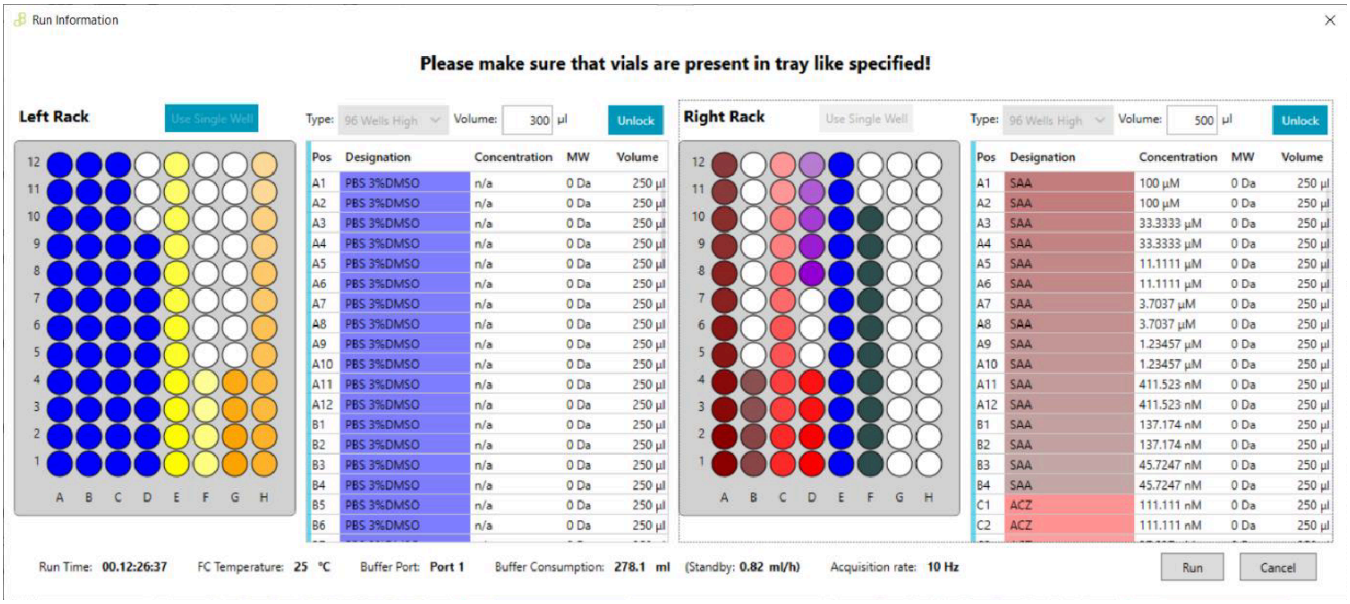


*Figure 6. Run window.*

○ It is possible to stop a process by hitting Queue and then Abort running or Abort All. Perform a prime after a process is aborted.

○ While creating a series, it is needed to fill up the Autosampler view (Figure 5), by filling up opportunely the different fields and positions. Two racks are usable (left and right), with three different rack types (48 vial adapter, 96 well plates, 384 well plates). **Only use vials and plates provided by the facility. Ask the Staff if you want or need to use your own plastics**.

## ➢ Results

○ **Save your data into the following pathway: OS (:C)/Users/Public/Creoptix/[GROUP_NAME]/[USER]/[Project_Name])**. A shortcut is available on the Desktop. **Note that this is a public folder, and the results are accessible to everyone. Do not modify or access other Users results. If you need to store the results into a different location (e.g. confidential data), please contact the Staff**.

## ➢ Evaluation

○ Results can be evaluated from the Evaluate&Simulate menu by selecting the desired option.

○ Kinetic data are automatically evaluated by clicking Evaluate&Simulate>Kinetic. The program automatically performs some adjustments and then evaluates the relevant kinetic and thermodynamic parameter.

- It is possible also to manually evaluate data:
  - Click on Evaluate&Simulate>Adjustement to manually define the different adjustments used in the evaluation (Jumps, Y-offset, X-offset, DMSO calibration, Blanks)
  - Click then on Evaluate&Simulate>Kinetic Analysis in order to run the evaluation with the selected Adjustments.
- In the Evaluation window (Figure 7) it is possible to modify several parameters used for the fitting, as well as to assess the quality of the fit. The user is referred to the manual for a more detailed description. In particular it is possible to use:
  - The Quality Panel (Figure 7): it assesses the quality of the fit, giving indications and evaluations on six different criteria (green=ok, blue=requires further verification, red=failed), suggesting possible next steps in case of failure.
  - The Evaluation Settings (Figure 8), which allows to define several settings (e.g. exclude some curves, choose among different binding models, use a traditional fit) used in the evaluation.

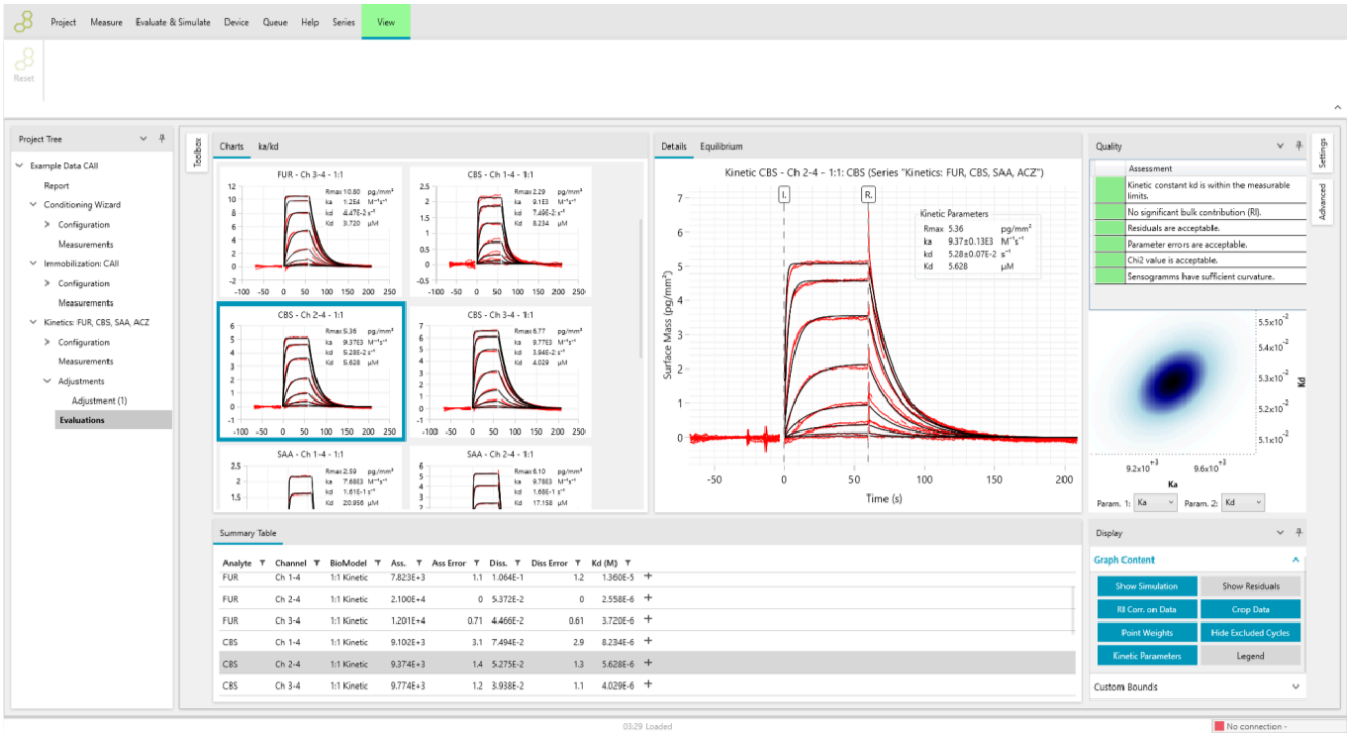


*Figure 7. Evaluation window. Quality Panel is depicted on the right.*

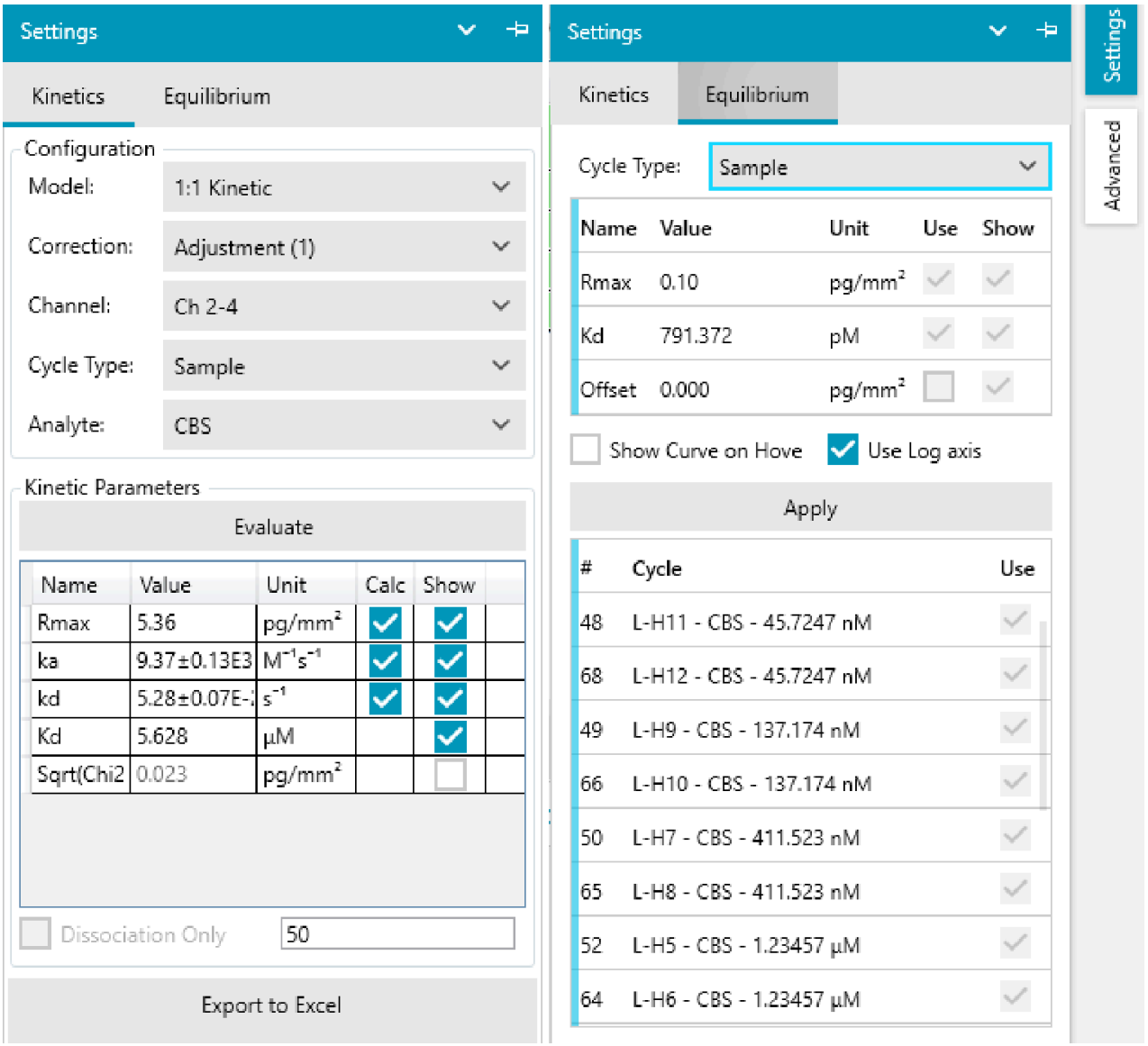


*Figure 8. Evaluation settings.*

## ➢ Reports

- Graphs can be added by choosing Add to report or Configure and Export.
- To export a report (Figure 9):
  - Select which series to export
  - Select a template
  - Click Export as pdf or Export as Word

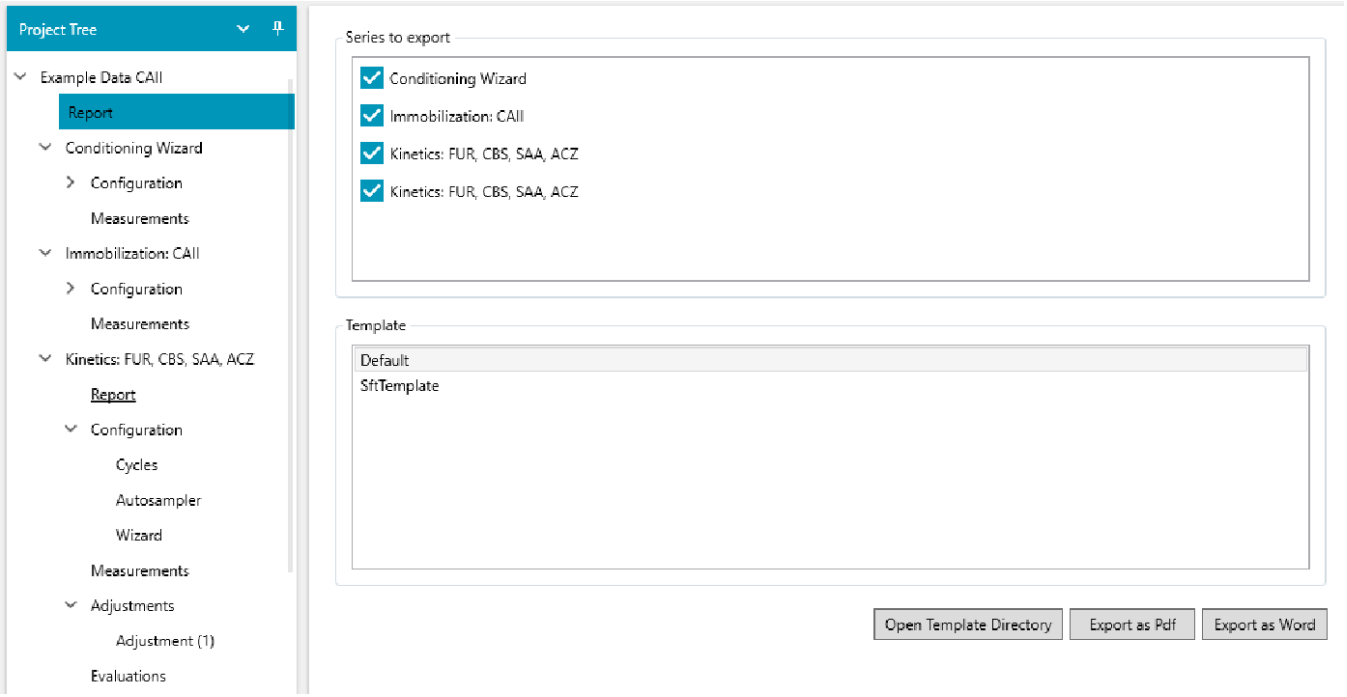


*Figure 9. Main report configuration window.*

## ➢ Help

- Please refer to the complete manuals, available also in the PC, for a complete description of the functions.
- For any issue, please contact the Staff.