

Quick Reference How-To Guide for the Olis DSM CD Models

Turning on the Olis DSM CD

- 1 Turn on the lamp cooling box.
- 2 Turn on the nitrogen flow to the lamp and monochromator to at least 6 L per min. *Higher flow rates in the monochromator should be used if data are to be taken before 200 nm.*
- 3 Turn on the power supply for the lamp.
- 4 Press and hold the ignite button until lamp ignites. *Ensure that the current to the lamp does not exceed 7.5 Amps.*
- 5 Turn on the main power switch at the power strip.
- 4 Turn on the computer and open GlobalWorks program.
- 5 Select the **Data Collection** tab and double click on **Conv CD**.
- 6 The spectrophotometer will initialize and calibrate.

Changing CD units of data collection

- ▶ One may choose from several units of data collection in the **Parameters** tab under **CD Units**.

Milliabsorbance: Reports data as the difference in absorbance of left circularly polarized light and right polarized light. ($Abs_{Left} - Abs_{Right}$)

Molar Extinction: Reports the difference in extinction coefficients for left and right polarized light. ($\epsilon_{Left} - \epsilon_{Right}$)

Millidegrees: Reports ellipticity in units of millidegrees..

Molar Ellipticity: Reports molar ellipticity in units of deg cm²/dmol. The user must provide the program with protein concentration (g/L), cell pathlength (cm), and mean residue weight (g/mol).

Taking a wavelength scan

- 1 Open the **Operational Modes** tab and set the **Data Collection Mode** to **Scan**.
- 2 Ensure that the proper **Data Reduction Mode** is selected (i.e., **Circular Dichroism**).
- 3 Go to **Live Display** tab.
- 4 Change **Wavelength Scan Range** to desired range.
- 5 Click on **Live Mode** button and adjust **PMT HV** value to give an acceptable signal (If you have photon counting you cannot change **PMT HV**).
- 6 Enter the desired number of increments to be collected and the integration time for each point.
- 7 Click on the **Collect Data** button to begin scan.

Taking repeated scans

- 1 Under **Repeated Scans** tab, change **Number of Scans** to the desired number. Scans can be made automatically as a function of time, or manually. In the **Auto** mode, the time selected is the total time to complete all scans. In the

Manual mode, scans are started by pressing the spacebar.

- 2 Select **Manual** or **Auto** as the **Scan Mode** on this page.
- 3 Ensure that **Time Units** are correct. These can be changed in the **Operational Modes** tab.
 - ▶ All repeated scan data will be saved as a single, 3-D data set.
 - ▶ Selecting **Average Scans** results in an output of a single, averaged scan.

Taking repeated scans as a function of a temperature script

- 1 In the **Repeated Scans** tab, select the desired temperature script by entering or browsing to the correct file.
- 2 To edit a script file, click on **Edit Script** and change the number of scans, temperatures and integration times.
- 3 Check that the temperature controller is set to **On** in the **Temperature Control** tab.
- 4 In the **Repeated Scans** tab, set **Repeat Scans as a function of to Temperature Script**. *The **Number of Scans** value should change to be equal to the number of scans in the temperature script.*
- 5 Select appropriate data collection parameters in the **Live Display** and **Operational Modes** tabs.
- 6 Click on **Collect Data** to begin Scans.

Taking an assay

- 1 Under the **Operational Modes** tab, set the **Collection Mode** to **Assay**.
- 2 Enter **Total Assay Time** in the **Live Display** tab.
- 3 Set **Current Wavelength** to the desired assay wavelength.
- 4 Enter **Number of Points to Collect** and **Integration Time** per data point.
- 5 To subtract an offset from the data, click on the **Zero Instrument** button.
- 6 To begin the assay, click on the **Collect Data** button and press spacebar when prompted.

Collecting repeated scans as a function of a titrator script

- 1 In the **Repeated Scans** tab, set **Repeat Scans as a function of to Titrator Script**.
- 2 Follow instructions for calibration.
- 3 Load solution into titrator using the **Titrator Control Panel** to move syringes.
- 4 To edit a script file, click on **Edit Script**.
- 5 Select appropriate data collection parameters in the **Live Display** and **Operational Modes** tabs.
- 6 Click on **Collect Data** to begin Scans.

Fitting 2-D data set

- 1 Click on dataset to be fit.
- 2 If you desire to fit only a portion of this data, select **Create Data Subset** in the **Tools** menu. When prompted, enter the desired range. Click on new dataset to select it.
- 3 Select **2-D Fits** under the **Fits** menu and select the desired model to fit the data. *If you would like a data fitting model added to the software, please contact Olis.*

Fitting a 3-D data set

- ▶ There is a tutorial under the **Help** menu which describes SVD data processing and fitting.

Changing the axis scale on a data set

- 1 Select desired data set
- 2 Right-click on graph
- 3 Select scale and enter desired values.

Viewing more than one set of data

- 1 Open all desired sets of data.
- 2 Select a dataset to be viewed (move between data sets in the **Experiments** window on the right).
- 3 Select **Copy Slice** under **Edit** menu.
- 4 Select second data set to view.
- 5 Select **Paste Slice** under **Edit** menu
 - ▶ To hide a slice from view (and from the printer), select it and select **Hide Slice** under the **View** menu.
 - ▶ To switch between hidden slices and viewed slices, select **Swap Hidden/Unhidden Slices** under **View** menu.

Smoothing a scan

- 1 In the **Experiment** window, select a dataset by clicking on it.
- 2 Right click on the desired dataset and choose **Select** from the pop up menu.
- 3 Right click on the dataset again and choose the **Smooth** option under **Data Processing** in the pop up menu.
- 4 Choose the degree of smoothing (3-25 points per average).
- 5 A new smoothed dataset will be generated in the **Experiment** window. The name will by default be “[original data file name]-smoothed.”

Smoothing a 3D dataset using SVD

- 1 Click on the desired dataset in the **Experiment** window.
- 2 Click on **SVD** to generate the SVD eigenvectors.
- 3 Choose **Reconstruct 3D from SVD Data**.

Naming a dataset

- 1 Double click on the **Name** property in the **Properties** window.
- 2 Enter a name for the dataset.
- 3 Press enter to assign the name. *This name will remain with the dataset and is distinct from the file name.*

Saving a dataset

- 1 Click on the desired dataset in the **Experiment** window.
- 2 Add any comments, and change the dataset name if desired.
- 3 Choose **Save Dataset** or **Save dataset as...** under the **File** menu. *Choose an appropriate directory and file name.*

Saving an experiment

- 1 Click on the desired experiment in the **Experiment** window.
- 2 Choose **Save Experiment** under the **File** menu.
- 3 The program will prompt for file names for each data set in the experiment. *When the experiment is reopened all the accompanying datasets will be opened.*

Assigning a baseline

- 1 Highlight the desired data set in the experiment window,
- 2 Left click on the data to select it and then right click on the data and select **Assign as Baseline**. *The baseline will continue to be applied until the wavelength range, number of data points, or Assign baseline checkbox have been changed.*

Exporting a 2-D data set

- 1 Select a data set to be exported.
- 2 Right click on the chart and select **Save as Ascii**.
- 3 Enter the filename when prompted.
 - ▶ Alternatively, data can be exported directly into Excel by selecting **Export to Excel** under the right-click menu.

Doing math on a dataset

- 1 In the **Experiment** window, select a dataset by clicking on it.
- 2 Right click on the dataset and choose **Select**.
- 3 Repeat this procedure for any datasets to be included in the mathematical operation.
- 4 Right click on the dataset again and choose the desired mathematical operation under the **Data Processing** menu. *These options are also available under the **Tools** menu.*
- 5 The new mathematically manipulated dataset will be generated in the **Experiment** window.

Converting CD units

- 1 Select data by clicking on icon in **Experiment** window and choosing **Select**.
- 2 Right click again and choose **Convert CD Units** under **Data Processes**.
- 3 Choose the appropriate units.

Printing a data set as a report

- 1 Select chart by clicking on dataset.
- 2 Select **Print Preview** under **File** menu and choose **Color** or **Black and White**.
- 3 Click on **Print**.

Pasting a dataset into Microsoft Word

- 1 Select chart by clicking on dataset.
- 2 Select **Send Chart to Clipboard** under **Chart** tab.
- 3 Open Microsoft Word document.
- 4 Choose **Paste Special** under **Edit** menu.
- 5 Double click on graph to edit it using Microsoft Draw.

Turning off the DSM CD instrument

- 1 Exit the GlobalWorks software by selecting **Exit** under the **File** menu.
- 2 Exit Windows and turn off main power switch.
- 3 Turn off power to lamp.
- 4 Turn off nitrogen flow.
- 4 Leave lamp cooling box on for a few minutes to help cool the lamp.

Deleting a slice from a dataset

- 1 Left click on a dataset to highlight it.
- 2 Choose **Edit Dataset** under the **Edit** menu.
- 3 Click on **Edit Axis Data** of the axis of the slice to remove.
- 4 Left click axis points or drag mouse to select multiple points.
- 5 Right click and select **Remove Axis Points** under **Axis Options**.
- 6 Click on **Save Axis Data**.
- 7 Click **Post Data to GlobalWorks**.

Changing the axis titles on a dataset

- 1 Left click on a dataset to highlight it.
- 2 Choose **Edit Dataset** under the **Edit** menu.
- 3 Change axis title and units. *Axis values can be changed by clicking **Edit Axis Data**, changing axis values, and clicking **Save Axis Data**.*
- 4 Click **Post Data to GlobalWorks**.

Building a 3-D dataset

- 1 Collect individual 2-D traces to be included in 3-D dataset.
- 2 Click on dataset.
- 3 Choose **Edit Dataset** under **Edit** menu.
- 4 Change Y axis title and units to new axis.
- 5 Repeat for each trace to be included. *Cut and paste may be used.*
- 6 Select all datasets to be included by right clicking each in the **Experiment** window and choosing **Select**.
- 7 Right click on a dataset in the **Experiment** window, choose **Build 3-D from 2-D** under **Data Processes**.
- 8 Select all datasets to be included by right clicking each in the **Experiment** window and choosing **Select**.
- 9 Click on the new dataset, choose **Edit Dataset** under the **Edit** menu.
- 10 Choose **Edit Axis Data**, enter new values and click **Save Axis Data**.
- 11 Click **Post Data to GlobalWorks**.

