

Quick Reference How-To Guide for the Olis Cary Models

Turning on the Olis modernized Cary spectrophotometer

- 1 Turn on the main power switch at the power strip.
- 2 Ensure that the control box and appropriate lamp(s) are on.
- 3 Turn on the computer and open Globalworks program.
- 4 Choose **Data Collection** and select the Cary icon.
- 5 Click **Open**.
- 6 The spectrophotometer will initialize and calibrate.

Changing data reduction modes

- ▶ Choose from the following in the **Operational Modes** tab under **Data Reduction Modes**:

Absorbance: Reports sample and reference signals as $\log(\text{ref}/\text{sam})$

Transmittance: Reports sample and reference signals as sam/ref

% Transmittance: Reports sam/ref as a %.

Reflectance: Reports sam/ref for reflective samples

Single beam: Reports sample and reference signals

Raw signals: Reports sample and references signals before dark signal is subtracted.

Adjusting PMT sensitivity

- ▶ In all modes of detection, the PMT high voltage is adjusted by clicking on the **PMT HV** value in the **Live Display** tab. *The higher this number, the larger the signal and accompanying noise will be.*
- ▶ In all modes except **Single beam** and **Raw signals**, the slit width will be adjusted automatically to keep the light intensity relatively constant. The higher the **PMT HV**, the smaller the slit width will be, resulting in noisier spectra with better spectral resolution.
- ▶ In the **Single beam** and **Raw signal** modes, the slits and **PMT HV** are adjusted by the user.

Adjusting detector sensitivity in the near infrared (NIR) range

- ▶ In all modes, the **NIR Gain** can be adjusted from 0.004 to 1. The lower this value, the higher the spectral resolution and noise.
- ▶ The **NIR Bias** is always adjusted automatically.
- ▶ In all modes except **Single beam** and **Raw signals**, the slit width will be automatically adjusted to keep the light intensity somewhat constant. The lower the **NIR Gain**, the smaller the slit width will be, resulting in noisier spectra and better spectral resolution.
- ▶ In the single beam and raw signal modes, **Slits** and **NIR Gain** are adjusted by the user.

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 (ie. **Absorbance**, **Transmittance**, etc.).
- 3 Go to **Live Display** tab.
- 4 Change **Wavelength Scan Range** to desired range (click on the number to highlight).
- 5 Enter values for **Number of Points to Collect** and **Reads per Datum** (the higher this number is the better the signal to noise ratio, but the longer the scan will take).
- 6 Click on the **Collect Data** button to begin scan.

Taking repeated scans

- 1 Under the **Repeated Scans** tab, change **Number of Scans** to the desired number.
- 2 Select **Manual** or **Auto** in the **Scan Method** box. *Scans can be made automatically as a function of time, or manually. In **Auto** mode, the time selected is the total time to complete all scans. **Manual** scans are started by hitting the spacebar.*
- 3 Ensure that **Time Units** are correct. *These can be changed in the **Operational Modes** tab.*
- 4 All repeated scan data will be saved as a single, 3-D data set.

Taking an assay (time drive)

- 1 Under the **Operational Modes** tab, set the **Collection Mode** to **Assay**.
- 2 Enter **Total Assay Time** in the **Live Display** tab.
- 3 Enter **Assay Wavelength**.
- 4 Enter **Number of Points to Collect** and **Integration Time**.
- 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.

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 range of the dataset you wish to fit. 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.

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**.

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**.

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.

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.*

Smoothing a data set

- 1 Highlight the data set in the **Experiment** window.
- 2 Left click to highlight the data and then right click on the data.
- 3 Select **Digital Filter** in **Data Processing** menu.
- 4 Select the appropriate (5-25 point) smooth.

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**.

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.

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.*

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.

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.

Turning off the Cary instrument

- 1 Exit the Globalworks software by selecting **Exit** under the **File** menu.
- 2 Exit Windows and turn off main power switch.

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.

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**.