Introduction

T-App is a computer program used to communicate with and control a Quantum Northwest (QNW) temperature-controlled sample holder. When **T-App** is run, it automatically connects to and begins communicating with a properly installed and connected QNW temperature controller (**QNW-TC**).

T-App can then be used to:
    control magnetic stirring (on, off and speed);
    turn temperature control on/off;
    set the target temperature (TT) which tells the **QNW-TC** the temperature desired;
    monitor of the sample holder temperature by presenting a plot of the temperature as a function of
        time;
    monitor the temperature measured with a series 400 thermistor probe connected to the **QNW-TC**;
        typically the thermistor probe is immersed in the sample to give an estimate of the sample
        temperature;
    save temperature data as a function of time to text files that can be loaded into other programs
        (such as Microsoft Excel) or into **T-App**;
    change the sample position for sample holders with multiple cuvette positions; and
    run a script which can contain an unlimited number of commands, issued sequentially, for control
        of the multiple capabilities.

T-App can be run in an Offline mode without a **QNW-TC**, primarily intended for loading and replotting data previously saved to files (for example, for comparison to other saved data).

T-App(S) is a version of **T-App** developed to communicate with a Shimadzu **UV-1800** absorbance spectrophotometer. It provides the user with additional capabilities:
    for single-cell sample holders,
        obtain and plot absorbance data as a function of temperature (melting, annealing),
        obtain and plot absorbance data as a function of time (kinetics),
        run simple absorbance scans as a function of wavelength;
    for multi-cell sample holders,
        obtain and plot multiple datasets as a function of temperature (or time),
        obtain and plot multiple datasets as a function of time at one or more constant
        temperature(s);
    for both sample holder types,
        copying or saving (as text files) the absorbance/temperature/time data that can be pasted into
        or loaded into other programs (such as Microsoft Excel) for replotting and manipulation.
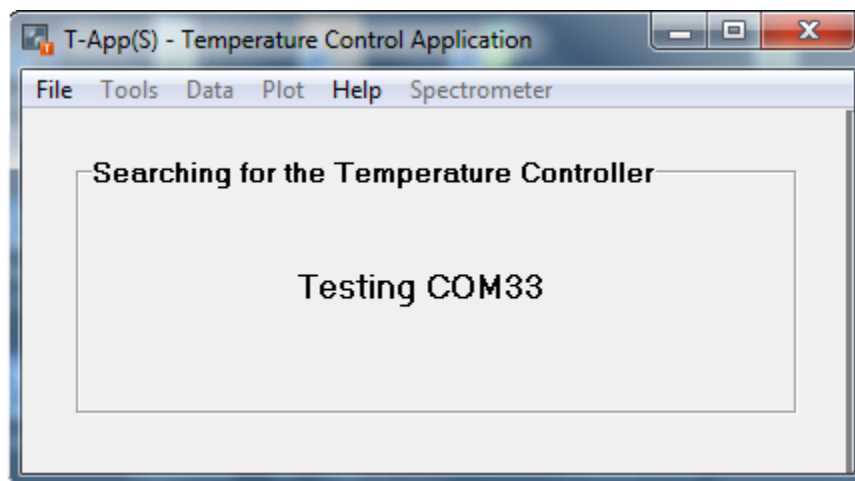
When **T-App(S)** is run in Offline mode, it can generate simulated temperature/absorbance data for single and 6-position sample holders. While originally introduced for debugging during program development, this simulation function can be helpful during training to demonstrate how the program

works and how to use the resulting text files for additional analysis. Many of the figures shown in this document were generated using Offline mode.
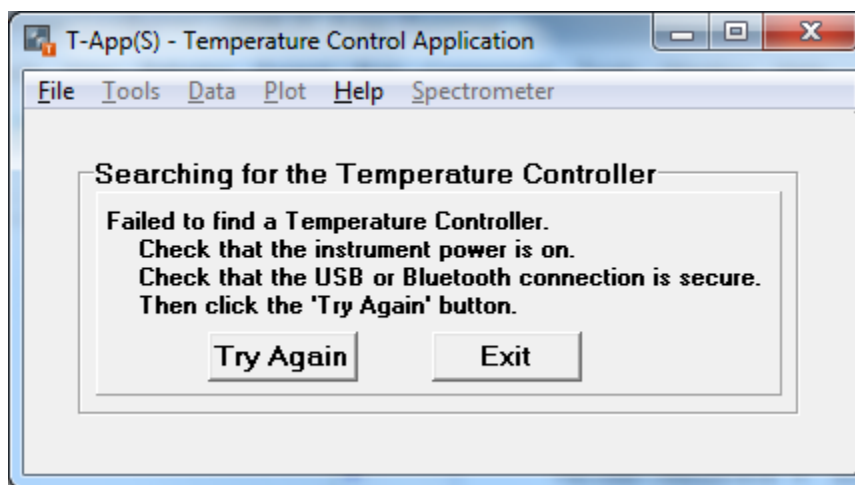
Except for the additional functionality with the Shimadzu **UV-1800**, the use of **T-App(S)** is identical to the use of **T-App**. Therefore, this document does not include extensive instructions for operating **T-App** beyond those needed for the enhanced capabilities defined above. See the **T-App** help file for complete instructions for using **T-App**.

T-App(S) startup windows

When **T-App(S)** is run, it begins testing all available COM ports to locate a **QNW-TC**. The window presented during this process is shown below.

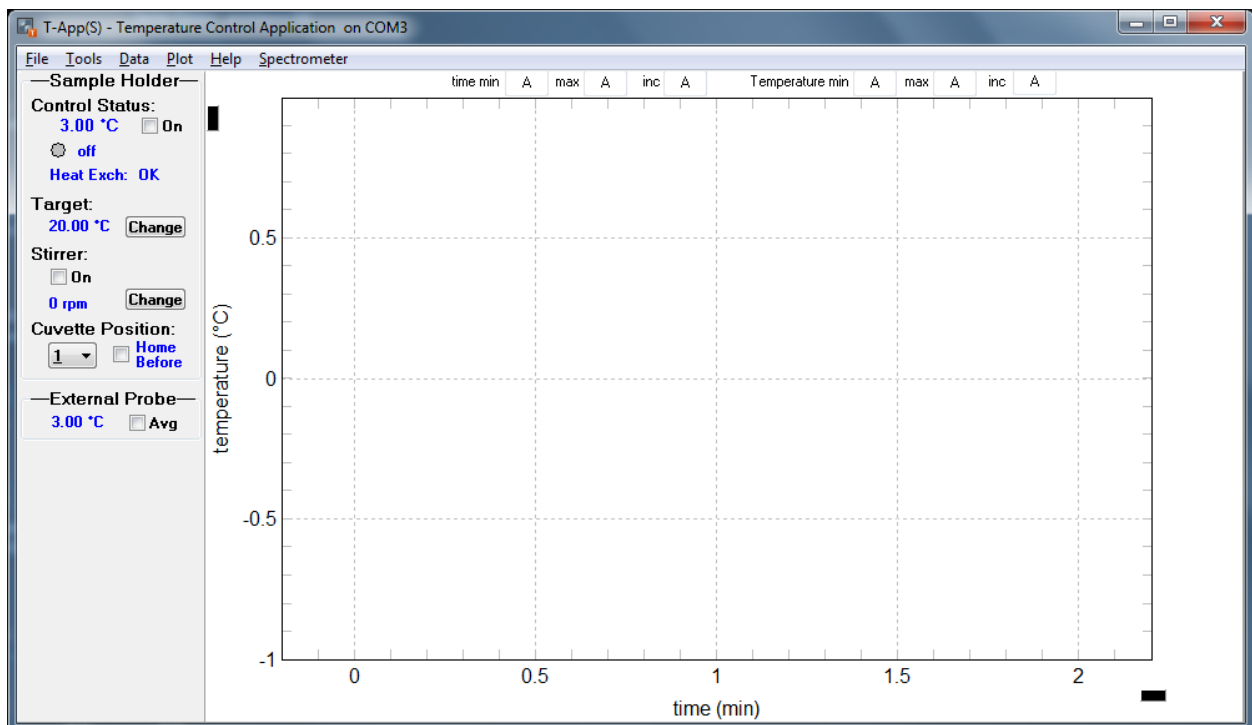If a **QNW-TC** is not found, the window changes to that shown below.

If connection to a **QNW-TC** was successful, the application window shown below will appear. The example shown is for a multi-cell sample holder with an external thermistor probe attached.

The gray rectangle on the left of the application window will be referred to as the Status Panel.

If no probe is attached, the External Probe section in the Status Panel will not be shown.

If you have a single-cell sample holder, the Cuvette Position section in the Status Panel will not be shown.

Note: the Work Offline menu item (see below) is not available in the File menu list once **T-App(S)** has connected to a **QNW-TC**. In this case you must close and reopen **T-App(S)** in order to work in offline mode.
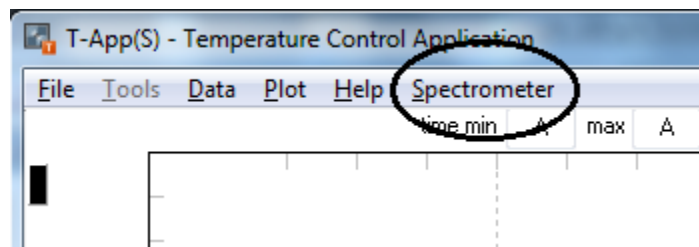
T-App(S) offline mode (data simulation mode).

To use the data simulation mode, run **T-App(S)** under conditions where it cannot connect with a **QNW-TC** (if a **QNW-TC** is connected to the computer, make sure its power is off). In the window presented, click on File in the menu bar and select Work Offline.

Then click on Spectrometer in the menu bar.

A second window will appear in front of the **T-App(S)** window. It will be titled Shimadzu UV-1800; it will be referred to below as the **UV-1800** window. The first (main) window will be referred to as the **T-App** window. The **UV-1800** window will stay in front even when you click on the **T-App** window. All of the menus and controls in the **T-App** window operate normally while the **UV-1800** window is visible and in front. However, it may sometimes be more convenient to hide the **UV-1800** window using the Hide Window button.   When the **UV-1800** window is not visible, data that has been or is being acquired will be available when it is made visible again by clicking on the Spectrometer menu item.

At the bottom of the **UV-1800** window, in the gray control panel, click on the Connect button. In offline mode the text control to the left of the button is usually blank unless the computer has a modem (in which case "COM3" may appear as shown here); in offline mode the content of this edit window is ignored.
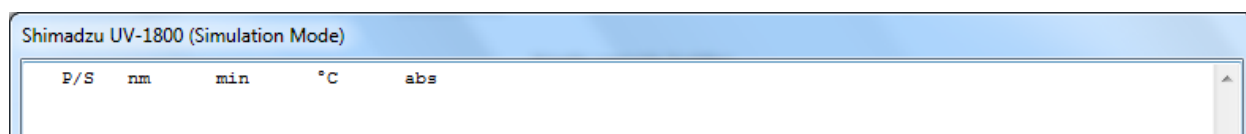
Clicking on the <u>Connect</u> button will cause the control panel to change as shown below.
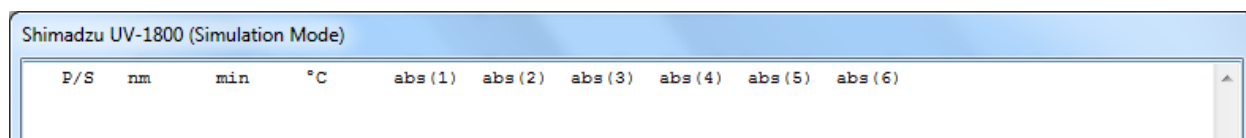

The button at the left end of the control panel will be enabled only when the <u>Sample Holder</u> and <u>Probe</u> check boxes to its right are both unchecked. Clicking on this button will clear the large data display above the control panel and toggle between the One Cell/Six Cell simulations. The header line at the top of the data display will indicate which simulation is currently selected as shown below.

One Cell simulation header

Six Cell simulation header

The <u>Load File</u> button shown above will change to a <u>Save Data</u> button whenever there is data in the large data display window above the status bar. If you clear the data by clicking on the <u>Six Cell</u> /<u>One Cell</u> toggle button, the caption will change back to <u>Load File</u>. Clicking on the <u>Save Data</u> button will bring up a <u>Save Dialog</u> to allow you to save the data in the display window to a text file. Clicking on the <u>Load File</u> button will bring up an <u>Open Dialog</u> where you can select a text file (which must have been created in the **UV-1800** window of **T-App(S)**) to be loaded.

To start a simulation, click on either the <u>Sample Holder</u> or the <u>Probe</u> check box. In the **T-App** window a plot of temperature as a function of time will begin (black is sample holder temperature, red is probe temperature). This simulation is for a temperature ramp at 1 $^\circ$C/min with temperatures reported every 6 seconds (0.10 min); the simulation is accelerated by a factor of 6 so that the 14 min simulation can be completed in 2-1/3 minutes. As is typical for a real temperature ramp, the probe temperature (measured with a thermistor immersed in the stirred sample and connected to the **QNW-TC**) lags behind the sample holder temperature.

A line of data is added in the data window each time a the temperature selected is received. If only one of the checkboxes is checked, the line specifies which by the 'S' or 'P' in the first column. If both the

Sample Holder and the Probe check boxes are checked, the data lines will be for probe temperatures only. If you uncheck both checkboxes, data will stop coming in; if you later recheck a box, data collection will resume but there will be missing lines because the simulation continues until it is either finished or you cancel it by unchecking the Sample Holder/Probe checkboxes.

Single sample holder

Shimadzu UV-1800 (Simulation Mode)

P/S	nm	min	°C	abs
S	550.0	0.00	15.00	0.1030
S	550.0	0.10	15.10	0.1031
S	550.0	0.20	15.20	0.1032
S	550.0	0.30	15.30	0.1033
S	550.0	0.40	15.40	0.1034
S	550.0	0.50	15.50	0.1035
S	550.0	0.60	15.60	0.1036

For the 6-cell simulation, the cell position is changed every 6 seconds (going back to position 1 after position 6) and the absorbance is displayed in the corresponding abs(N) column.

6-cell sample holder

Shimadzu UV-1800 (Simulation Mode)

P/S	nm	min	°C	abs(1)	abs(2)	abs(3)	abs(4)	abs(5)	abs(6)
P	550.0	0.00	15.00	0.1030					
P	550.0	0.10	15.10		0.1110				
P	550.0	0.20	15.20			0.1170			
P	550.0	0.30	15.30				0.1210		
P	550.0	0.40	15.40					0.1230	
P	550.0	0.50	15.50						0.1240
P	550.0	0.60	15.60	0.1036					
P	550.0	0.70	15.70		0.1110				
P	550.0	0.80	15.80			0.1170			
P	550.0	0.90	15.90				0.1210		

When the 6-cell simulation is running in the **UV-1800** window, the **T-App** window shows (on its right side) the controls needed to run and monitor a script. As the simulation runs, the commands and controller responses that would be seen with such a script are simulated in the large text display as shown in the adjacent figure. The script file itself (a simple text file) that would be used to control this process is shown at the far right.

```
...[F1 PT 17.40]
[F2 PL 2]
...[F2 DL 2]
[*D 8]
[F1 PT ?]
...[F1 PT 17.50]
[F2 PL 3]
...[F2 DL 3]
[*D 8]
[F1 PT ?]
...[F1 PT 17.60]
[F2 PL 4]
...[F2 DL 4]
[*D 8]
[F1 PT ?]
...[F1 PT 17.70]
[F2 PL 5]
...[F2 DL 5]
[*D 8]
[F1 PT ?]
...[F1 PT 17.80]
[F2 PL 6]
...[F2 DL 6]
[*D 8]
```

☐ Show Script Comments

Run Script File

Clear Display

Controller Script
Interval = .6
[F2 DL 1]
[*D 8]
[F1 PT ?]
[F2 DL 2]
[*D 8]
[F1 PT ?]
[F2 DL 3]
[*D 8]
[F1 PT ?]
[F2 DL 4]
[*D 8]
[F1 PT ?]
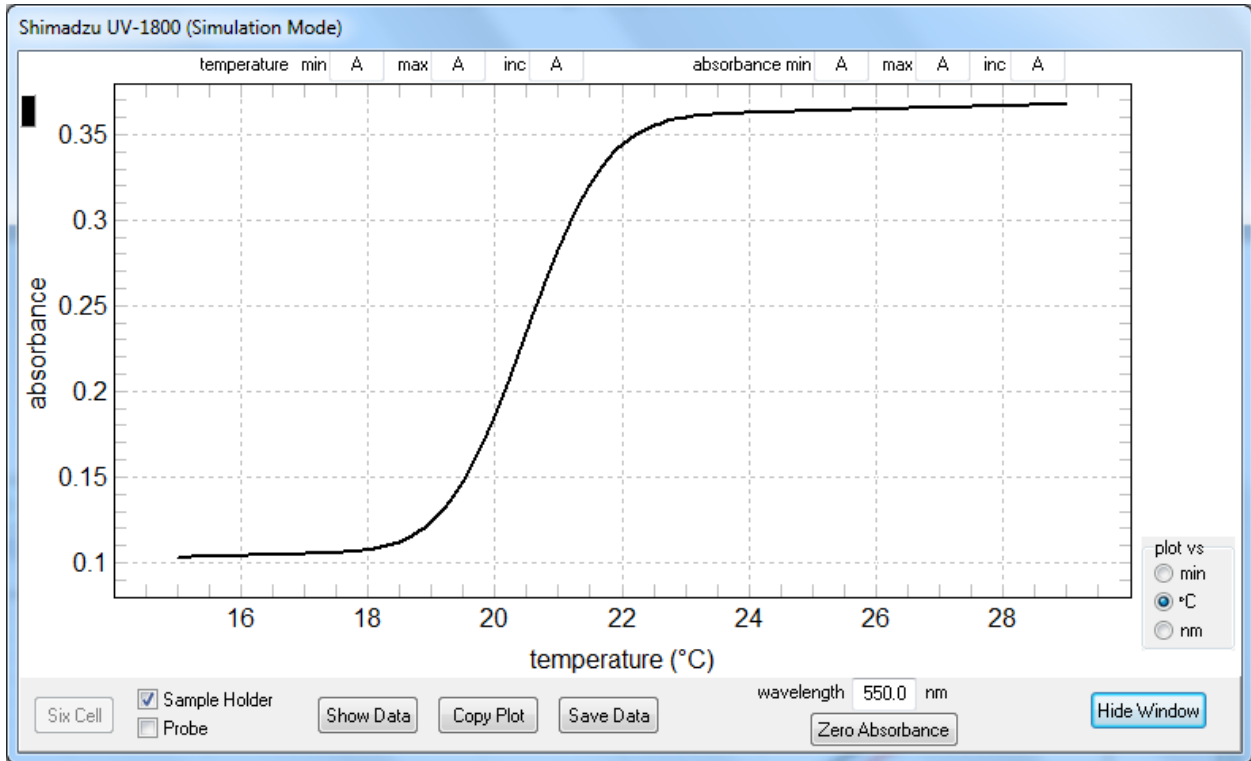[F2 DL 5]
[*D 8]
[F1 PT ?]
[F2 DL 6]
[*D 8]
[F1 PT ?]
[*R]

The results in the data display are tab-delimited to be consistent with commercial data analysis software (such as Microsoft Excel). You may select a range of data within the data window and copy it to the Windows clipboard by right clicking with the mouse cursor within the data window and selecting from the drop-down menu list presented. If the data listing is visible, the Copy Data button will copy all of the results accumulated (since the last time it was cleared) to the Windows clipboard. If the plot window is visible, the Copy Plot button copies the plot (minus any controls) to the clipboard. The Save Data button provides a means of saving the data to a text file (whether the data or the plot is shown).

The content of the wavelength selection box in the bottom right of the **UV-1800** window determines the wavelength listed in each line of the data display lines under the heading "nm". Once you have changed the contents of this checkbox, you must hit the Enter key to complete the process. The Zero Absorbance button, just under the Wavelength box, has no effect in simulation mode.

Clicking on the Show Plot / Show Data button toggles between the two views. The plot examples below are for the completed One Cell and Six Cell simulations.

Completed One Cell simulation

Completed Six Cell simulation

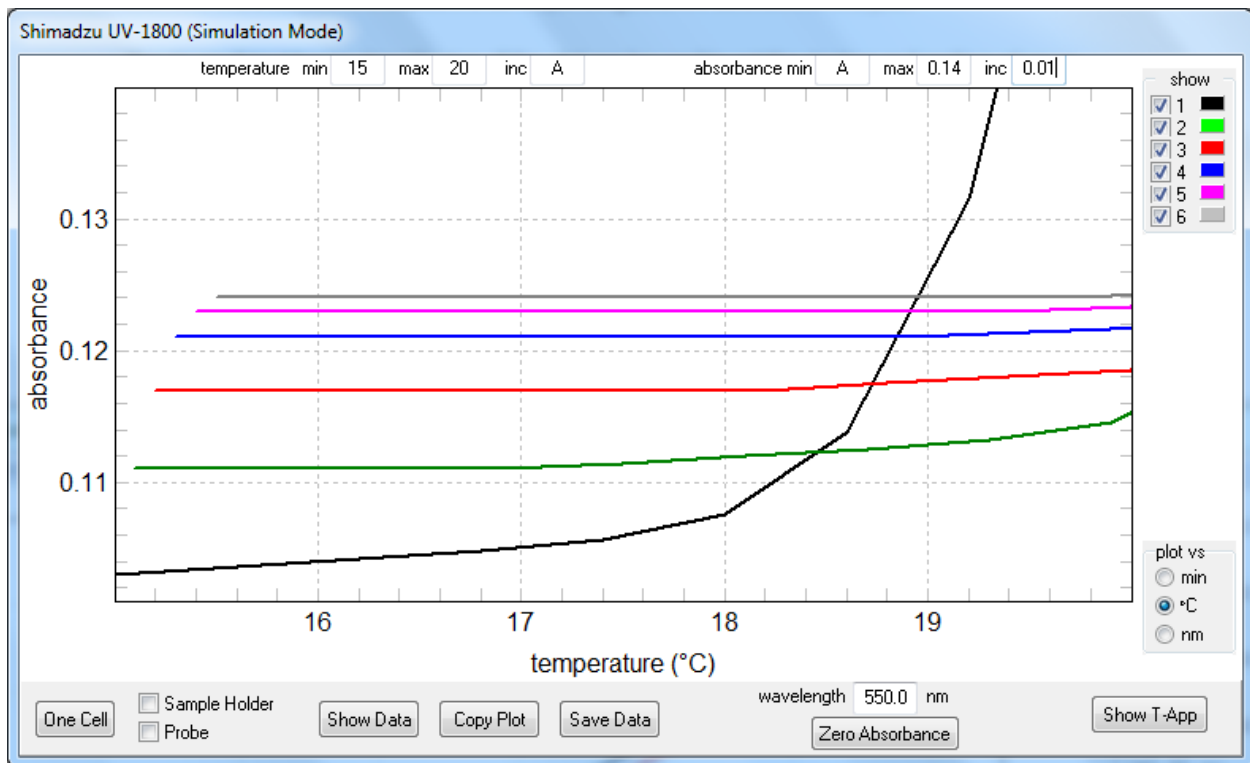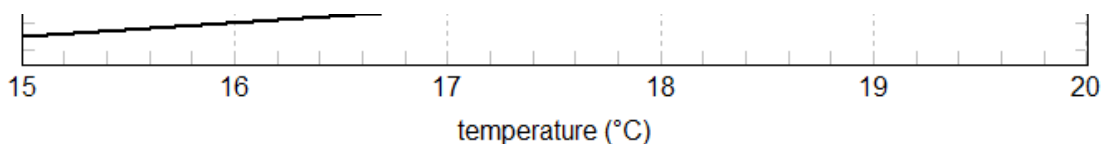The three radio buttons in the lower right corner of the plot can be used to change the horizontal axis variable to time (min), temperature (°C) or wavelength (nm). This change can be made at any time.

In the Six Cell simulation plot, the panel at the upper right of the plot includes one checkbox for each of the cell positions; each is coded for the cell number and the color of the line representing the data for that cell. If a checkbox is checked, the corresponding data will be shown in the plot.

The six small text boxes along the top of the plot can be used to set the starting and ending values as well as the tic increment to be used for each of the axes of the plot. An example, expanding the first part of the data on both axes, is shown below. If the entry is 'a' or 'A', that parameter is Automatically determined. Once a value has been entered, it takes effect (shows in the plot) when you hit the Enter key, the Tab key or otherwise activate a different control (such as clicking on one of the other range boxes, the Copy Plot button, the Sample Holder checkbox, etc.) by clicking on it.

If, for presentation, you would like the tic labels to include the corners of the plot, enter numbers that are very slightly smaller or larger. For example, for the temperature axis enter 14.999 and 20.001 as the min and max to give the result below (the plot, not the window, was copied and pasted for this illustration).

Using T-App(S) with the Shimadzu UV-1800

When a **UV-1800** spectrophotometer is equipped with a Quantum Northwest temperature controlled sample holder, it extends the instruments capabilities by permitting any measurement the **UV-1800** is capable of (absorbance, percent transmittance, energy) to be done at temperatures ranging from below 0 to above 100 ^oC. However, **T-App(S)** is designed for presentation only of absorbance data.

T-App(S) further enhances these capabilities by allowing the user to conveniently and automatically measure absorbance:
> for several discrete wavelengths at multiple stable sample temperatures;
> as a function of temperature using either a slow, linear (with time) temperature ramp or discrete
> > steps of the temperature;
> for single or multiple samples as a function of time at a stable temperature (e.g, enzyme assays or
> > other kinetics);
> for multiple samples as a function of temperature.

While use of **T-App(S)** does not require that the Shimadzu **UVProbe** software be properly installed on the computer to be used, the drivers required for **T-App(S)** to communicate with the **UV-1800** do have to be installed. The drivers required for **T-App(S)** to communicate with the **QNW-TC** will have been installed with **T-App(S)**.

The instructions provided below assume:

1. The Shimadzu **UVProbe** software (or just the required driver) has been properly installed on the computer to be used.
2. The **UV-1800** <u>square</u> USB socket is connected to the computer; if the **UVProbe** software is installed it should have been demonstrated to connect to and control the **UV-1800**.
3. The drivers for the **QNW-TC** serial communications chip have been installed. Either run the driver installation program (**CDM v2.12.04 WHQL Certified.exe**) provided with **T-App(S)** or this driver installation program can be downloaded directly from http://www.ftdichip.com/Drivers/VCP.htm.
4. The **QNW-TC** square USB socket is connected to the computer and the **T-App(S)** program has been demonstrated to connect to and control the **QNW-TC**.
5. The **UV-1800** has been turned on and has completed its startup sequence.
6. The **UVProbe** software <u>is not</u> running on the computer. If it is running then **T-App(S)** will not be able to connect to the **UV-1800**.
7. **T-App(S)** is running and has been connected to the **UV-1800** by clicking on the <u>Spectrometer</u> menu item in the **T-App** window and then clicking on the <u>Connect</u> button in the resulting **UV-1800** window. The connection should be tested by clicking on the <u>Sample Holder</u> checkbox; if lines do not begin appearing in the data window the connection has not been made (or automatic temperature reporting has been turned off in the **T-App** window.

Instruction for setup of the **UV-1800**.

1. Turn on the **UV-1800** spectrometer; wait until it completes the setup checks.
2. In the Mode menu display press 8. Then in the resulting Utilities display press 2 until the display line
    of that number reads Abs(4) %T(2). This causes absorbance values to have four digits after the
    decimal. Press RETURN to return to the Mode menu. While T-App will work fine with the three
    decimal digits setting, the spectrometer resolution is greater than that and slow changes in
    absorbance will show larger 'stair steps'.
    Note: This setting persists when the power is turned off and later back on.
3. Press F4 to put the **UV-1800** into PC Control mode.

Connecting **T-App(S)** to the **UV-1800**.

1. Turn the **QNW-TC** power on.
2. Start **T-App(S)**. When it connects to the **QNW-TC** the plot will begin to show sample temperatures
    within three seconds.
3. Click on Spectrometer in the menu bar.
4. In the **UV-1800** window that opens, select the proper COM number and click on the Connect button.
    Note: It is possible to do step 4 with the **UV-1800** not in PC Control mode and the program will
    connect to the spectrometer but will not be able to communicate with it. If this happens, click on the
    Clear button in the **UV-1800** window (the two checkboxes next to the Clear button must be
    unchecked to do this).
5. Click on the Sample Holder checkbox; lines of data should begin to appear within 3 seconds, spaced
    by 3 seconds (0.05 min). If this does not happen, see the note with step 4.

Instructions for setup of **T-App(S)** once it is connected to the **QNW-TC** and the **UV-1800**.

Note: Most of the example data included were obtained by running scripts which were usually designed
    to include all of the setup steps needed.   The instructions given here are steps that you would want
    to be familiar with in order to proceed without using a script. In the following, the functionality of
    T-App(S) will be accessed by means of the menu bar. Some steps can be performed using controls in
    the gray control panel at the left of the application window.
1. Set the desired target temperature. Click Tools in the menu bar and select Temperature Control,
    then select Set Target … . Or click on the Change button to the right of the word Target. In either
    case a Sample Holder Target Temperature parameter entry dialog will be presented.
Note: from this point on, sequences of menu selection will be represent in the form "click on
    Tools>(Temperature Control)>(Set Target …)".
2. Turn on temperature control. Click on Tools>(Temperature Control)>On. Or click on the **On**
    checkbox near the top of the status panel.
3. Turn on magnetic stirring. Click on Tools>(Stirrer Control)>On. Or click on the **On** checkbox under
    the word Stirrer in the status panel.

4. Change the stirrer rate (rpm). Click on <u>Tools>(Stirrer Control)>(Set Speed …)</u>. Or click on the <u>Change</u> button to the right of the word Stirrer. In either case a <u>Sample Stirrer Speed</u> parameter entry dialog will be presented. Note: when stirring is off, changing the stir speed turns it on.

5a. Change the cuvette position. Click on <u>Tools>(Cuvette Position)>N</u>. Or click on the arrow of the drop-down list under the words Cuvette Position in the status panel and chose one of the numbers in the list. The carrier will move to the selected position.

5b. "Home" the cuvette holder (go to an alignment location) before setting the selected position. Click on <u>Tools>(Cuvette Position)>(Home Before)</u>. Or click on the <u>Home Before</u> checkbox in the control panel.

6. Start a linear temperature ramp. Click on <u>Tools>(Temperature Ramping …)</u>. A <u>Ramping parameters</u> entry dialog will be presented. The <u>End (^{o}C)</u> is the temperature to ramp to (the ramp Target Temperature). The <u>Rate (^{o}C/min)</u> parameter determines the slope of the ramp. When the <u>OK</u> button is clicked, the temperature will begin changing from the current temperature to the ramp target temperature at the specified rate. While there is no lower limit to the ramp rate, high rate settings may result in non-linear results because the system will eventually reach a point where it cannot change the temperature at the specified rate.

7. To run a script, click <u>Tools>(Show Script Panel)</u>. This will cause a vertical panel to open at the right side of the **T-App** window with controls for selecting a script file to be run. Select <u>Tools>(Hide Script Panel)</u> to close it.

8. To send individual commands to the **QNW-TC**, click on <u>Tools>(Show Command Panel)</u>. This will cause a vertical panel to open at the right side of the application window with controls for entering and sending commands. The large text control (display window) will display the commands when sent and will display any replies returned by the **QNW-TC**. Select <u>Tools>(Hide Command Panel)</u> to close it.

9. When **T-App(S)** starts, it instructs the **QNW-TC** to begin sending temperature reports at 3 second intervals that appear in the temperature plot. The three temperatures are CT (the sample holder temperature, black), HT (the heat exchanger temperature, blue – see 11 below) and PT (the external probe temperature, red). The latter (PT) will be available only if an external probe is connected to the **QNW-TC**. The user can stop automatic reports by clicking on <u>Plot>Stop</u>. Clicking on <u>Plot>(Clear & Restart)</u> will clear the plot, restart the time at 0, and tell the controller to restart sending temperature reports. Clicking on the <u>Plot>(Clear All)</u> will just clear the plot but not reset the time.

10. To change the interval between automatic temperature reports, click on <u>Plot>(Time Interval …)</u>. A <u>Plot Time-Interval</u> entry dialog will be presented; the lower limit for the interval is 1 second; there is no upper limit.

11. Click on <u>Plot>(Data Shown)>(Sample</u> or <u>Probe</u> or <u>Heat Exchanger)</u> to determine if the respective temperature is to be shown in the plot. A checkmark next to the menu item indicates that that temperature will be included in the plot.

12. Click on <u>Plot>Copy</u> to copy the plot to the clipboard.

13. Click <u>Data>Copy>(Sample Holder</u> or <u>Probe</u> or <u>Heat Exchanger)</u> to copy the respective data in tabbed text form to the clipboard.

14. Click <u>Data>Save>(Sample Holder</u> or <u>Probe</u> or <u>Heat Exchanger)</u> to save the respective data in tabbed form to a text file.

15. Click <u>Data>(Load from File into)>(Sample Holder</u> or <u>Probe</u> or <u>Heat Exchanger)</u> to open a file that has been saved from the **T-App** window and load the data into the selected data location.

Click on <u>Spectrometer</u> in the menu bar to show the **Shimadzu UV-1800** window.

1. In that window, click on the arrow to the left of the <u>Connect</u> button and, from the drop-down list, click on the COM number for the **UV-1800**, then click the <u>Connect</u> button.
   Note: If you do not know which is correct, write down the numbers for the entries in the list; then close **T-App(S)**. Unplug the USB cable from the **UV-1800** at the computer and restart **T-App(S)**. Again, click on <u>Spectrometer</u> and examine the list again; make a note of which of the numbers is missing; that will be the one for the **UV-1800**. Again close **T-App(S)**, reconnect the USB cable, restart **T-App(S)**, click on <u>Spectrometer</u>, select the correct entry from the list and click the <u>Connect</u> button.
2. If the connection is successful, the box containing the drop-down control and the <u>Connect</u> button will disappear and other controls will appear along the bottom of the window. If you do not have a thermistor probe connected, the <u>Probe</u> checkbox will be disabled (grayed).
   Note: You may close this window (by clicking on the <u>Hide Window</u> button in the lower right corner) and reopen it (by clicking on <u>Spectrometer</u>) at any time; any data already collected or still collecting will be unaffected.
3. Click in the <u>wavelength</u> text entry control and enter the wavelength desired. Then hit the Enter key and the **UV-1800** will slew to the chosen wavelength. You should do this (just click in the control and hit Enter) even if you want the program default wavelength of 550 nm (chosen because this is the default setting for the **UV-1800** on startup). **T-App(S)** has no way to determine what wavelength the **UV-1800** is set to (unless you set it here). *If at some point during a session you take the **UV-1800** out of the <u>PC Control</u> mode, it returns to 550 nm, so make a point of setting the wavelength in T-App(S) every time you return the **UV-1800** to <u>PC Control</u> mode.*
4. In the **T-App** window menu bar click <u>Plot>(Clear & Restart)</u> to make sure sample holder temperatures are coming in (see the note at the end of this paragraph). Then click on the <u>Sample Holder</u> checkbox in the **UV-1800** window. Now, each time a sample holder temperature is received a corresponding line will be written in the **UV-1800** window. This is the only mechanism for obtaining absorbance values provided by **T-App(S)**. That means, even if you only want to collect absorbance as a function of time or of wavelength, you must request a temperature in order to get it.
   Note: Clearing the **T-App** time/temperature plot will generally make seeing changes in the plot easier to see as new temperature values are added. However, a line will not appear on the plot until two temperatures differing by 0.01 have been reported, which may take a while if the sample holder temperature is stable. In this situation, you can still tell that temperatures are being reported because the horizontal axis maximum will change with each temperature received.
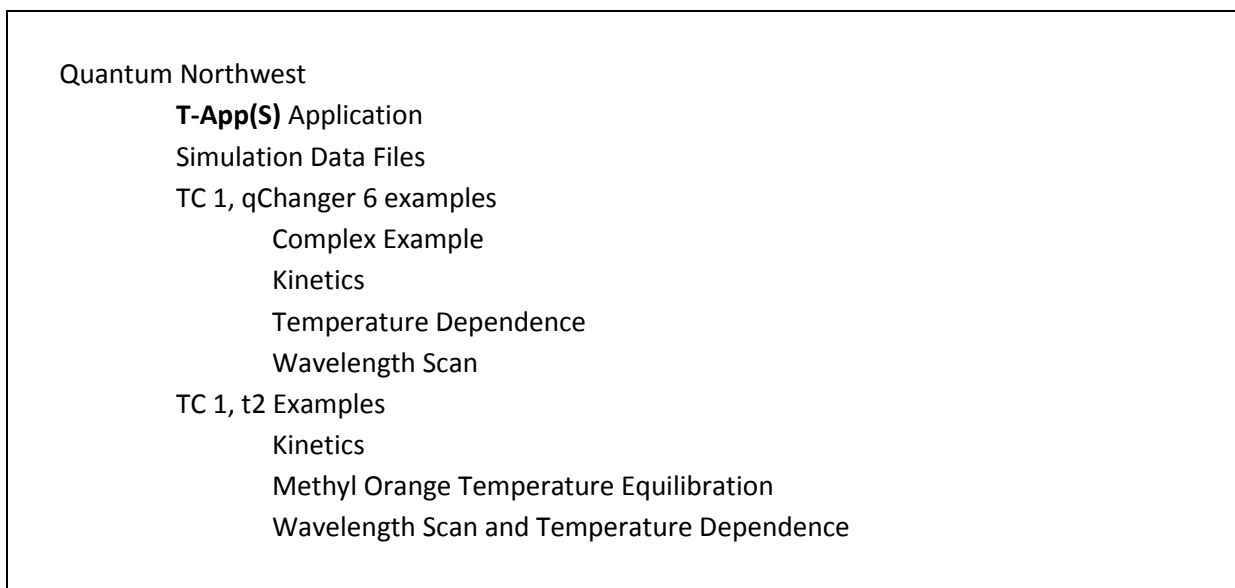
Non-Script Example: collect absorbance data every 5 seconds at a single wavelength for a single sample position during a temperature ramp.

The steps listed for the following method assume that **T-App(S)** is running and has successfully connected to the **QNW-TC** and to the **UV-1800**.

1. Click on <u>Plot>(Time Interval …)</u> In the parameter entry box, enter 5. If temperatures were not already being plotted, they will begin showing up now, five seconds apart.
2. Put a cuvette containing just the solvent in the sample holder (and one in the reference holder if required).
3. Set the wavelength desired.
4. Begin acquiring Sample Holder or Probe data (click the corresponding checkbox in the **UV-1800** window). Click on the <u>Zero Absorbance</u> button. Wait until a new data line appears to be certain that the auto zero process has finished.
5. Place your sample in the sample holder.
6. Click on <u>Tools>(Temperature Control)>(Set Target …)</u> In the parameter entry box. enter the starting temperature (such as 10 $^{\circ}$C).
7. Click on <u>Tools>(Temperature Control)>On</u>.
8. Click on <u>Tools>(Stirrer Control)>(Set Speed …)</u> In the parameter entry box, enter the desired speed (such as 500 rpm). Setting the stirring speed also turns stirring on.
9. Wait until the temperature stabilizes. The stirred sample takes longer than the sample holder temperature to stabilize. This will be readily apparent if you have a probe connected and immersed in the sample. Generally you should allow at least 5 minutes more after the sample holder temperature is stable.
10. If you have stopped, begin acquiring Sample Holder or Probe data.
11. Click on <u>Tools>(Temperature Ramping …)</u>. In the parameter entry box, enter the ramp rate (such as 1 $^{\circ}$C) and end temperature (such 30 $^{\circ}$C).
12. Click on <u>(Plot>Clear & Restart)</u>. This clears both the temperature plot in the **T-App(S)** window and the data (and plot) in the **UV-1800** window.
13. When the temperature reaches the ramp end, uncheck <u>Sample Holder</u> and/or <u>Probe</u>.
14. Save data, copy data, copy plot, etc., as needed.

Example scripts and data, obtained using T-App(S) with single and multiple sample holders.

This program is provided as a folder named <u>Quantum Northwest</u> that contains four subfolders, two of which have subfolders within them as diagrammed below.

```
Quantum Northwest
        T-App(S) Application
        Simulation Data Files
        TC 1, qChanger 6 examples
                Complex Example
                Kinetics
                Temperature Dependence
                Wavelength Scan
        TC 1, t2 Examples
                Kinetics
                Methyl Orange Temperature Equilibration
                Wavelength Scan and Temperature Dependence
```

The <u>Quantum Northwest</u> directory contains two files in addition to the four subfolders:
<u>Instructions.txt</u> that tells how to get the files onto the computer to be used.
T-App(S) <u>Manual.pdf</u>, which is this file.

The **T-App(S)** <u>Application</u> folder contains the program, **T-App(S)**.exe, the **T-App(S)** help file, and an executable used to install the drivers needed for serial communications between **T-App(S)** and the TC 1 (**QNW-TC**).

The <u>Simulation Data Files</u> folder contains data files saved after running the "One Cell" and the "Six Cell" simulations with **T-App(S)** in Offline Mode.

The <u>TC 1, t2 Examples</u> folder contains three subfolders:

<u>Kinetics</u> contains a script file used to monitor the kinetics of bleaching of blue food coloring at three wavelengths, the data resulting from running the script, and a pdf file that describes the experimental setup, the results, and a detailed description of the script commands used.

<u>Methyl Orange Temperature Equilibration</u> contains a pdf file describing manual (i.e., not script based) tests of temperature equilibration within a liquid sample of methyl orange as compared to temperature equilibration of the sample holder temperature reported by **T-App(S)**. The

directory also contains data files of absorbance as a function of temperature for rapid temperature changes between 20 and 60 ^{o}C.

Wavelength Scan and Temperature Dependence contains: a script file used to do a wavelength scan at 10 ^{o}C, monitor absorbance at two wavelengths as a function of a temperature ramp from 10 to 60 ^{o}C, and a wavelength scan at 60 ^{o}C; the data obtained; and a pdf file describing the experimental setup, the results, and a detailed description of the script commands used. The pdf file also provides detailed instruction for separating the data for the two scans from the temperature ramp data and for processing the temperature ramp data in Microsoft Excel to obtain useful plots of the results.

The TC 1, qCHANGER 6 Examples folder contains three subfolders:

Complex Example contains a script file which measures absorbance as a function of temperature, at five wavelengths for six samples. The temperature of the sample holder is changed in steps. A document file (pdf) describes the setup, the results, data manipulation in Microsoft Excel, and detailed description of the commands in the script. This is the most complex example of the use of **T-App(S)** in that three parameters are varied (wavelength, temperature and sample position).

Kinetics contains a script file used to monitor kinetics of bleaching of blue food coloring at five different concentrations of bleach; the data resulting from running the script; and a pdf file that describes the experimental setup, the results, and a detailed description of the script commands used. The document file also includes a description of how to use Microsoft Excel to take the complex data file and reduce it to individual data files that could be used for analysis of the transitions; the files that resulted are also included.

Temperature Dependence contains a script file used to monitor the absorbance at 260 nm of calf thymus DNA samples at five ionic strengths and the data resulting from running the script. There is also a pdf file describing the experimental setup, the results, and a detailed description of the script commands used. The document file also includes a description of how to use Microsoft Excel to take the complex data file and reduce it to individual data files that could be used for analysis of the transitions; the files that resulted are also included.

Wavelength Scan contains a script file used to do absorbance vs wavelength scans on 5 different food dye samples and the data resulting from running the script. There is also a pdf file describing the experimental setup, the results, and a detailed description of the script commands used. The document file also includes a description of how to use Microsoft Excel to take the data and reduce it to files containing only two columns (wavelength and absorbance) for possible analysis.