

Lesson 5: ITC Data Handling

Every data plot in Origin has an associated worksheet. The worksheet contains the X, Y and, if appropriate, the error bar values for the plot. A worksheet can contain values for more than one data plot.

It is always possible to view the worksheet from which data were plotted. This lesson shows you how to open the worksheet associated with a particular data plot, copy/paste the data, export the data to an **ASCII** file, and import **ASCII** data.

Reading Worksheet Values from Plotted Data

Begin this lesson by opening the ITC **Rnahhh.ITC** data file series, as follows:



Shortcut: Select the New Project button.

- Select **File : New : Project**.
A new Origin project opens to display the **RawITC** plot window.
- Click on the **Read Data..** button.
The File **Open** dialog box opens, with the **ITC Data (*.IT?)** file name extension selected.
- If you have not previously **Set Default Folder...** to the samples folder, then navigate to the C:\Origin70\samples folder.
- Select **Rnahhh** from the file name list, and click **OK**.

As you saw in Lesson 1, Origin plots the **Rnahhh** data as a line graph in the **RawITC** plot window, automatically creates a baseline, integrates the peaks, normalizes the integration data, and plots the normalized data in the **DeltaH** plot window. As a result, the following eight data sets are created:

rnahhh_dh	Experimental heat change resulting from injection <i>i</i> , in $\mu\text{cal/injection}$ (not displayed).
rnahhh_mt	Concentration of macromolecule in the cell <i>before</i> each injection <i>i</i> , after correction for volume displacement (not displayed).
rnahhh_xt	Concentration of injected solute in the cell <i>before</i> each injection (not displayed).
rnahhh_injv	Volume of injectant added for the injection <i>i</i> .
rnahhh_ndh	Normalized heat change for injection <i>i</i> , in calories per mole of injectant added (displayed in DeltaH window).
rnahhh_xmt	Molar ratio of ligand to macromolecule after injection <i>i</i> (X value of data point).
rnahhhbase	Baseline for the injection data (displayed in red in the RawITC window).
rnahhhraw_cp	All of the original injection data (displayed in black in the RawITC window).

In addition origin creates two temporary data sets:

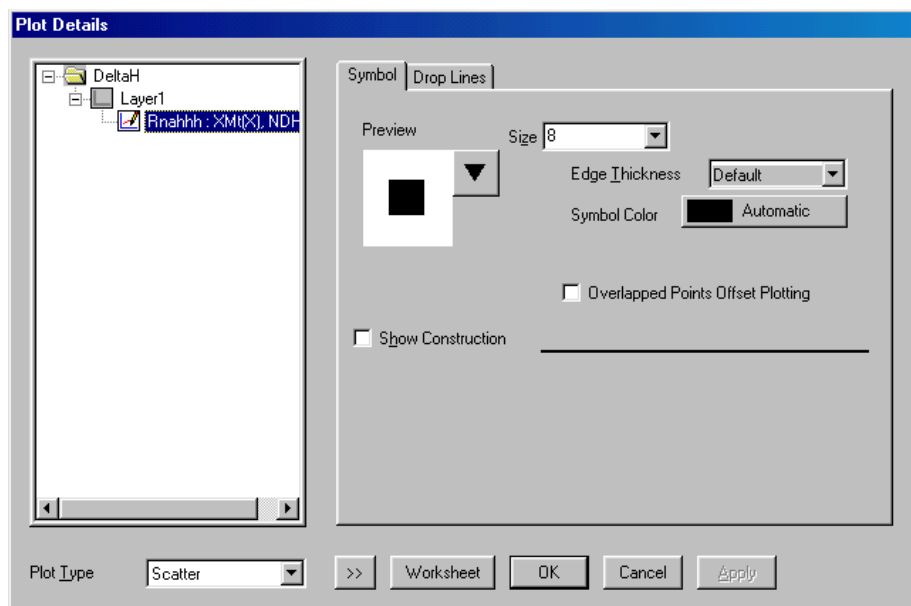
rnahhhbegin	Contains the indices (row numbers) of the start of an injection.
rnahhhrange	Contains the indices of the integration range for the injections.

An Origin data set is named after its worksheet and worksheet column, usually separated by an underscore. Thus the first six data sets above will all be found on the same worksheet (**RNAHHH**), in columns named **DH**, **INJV**, **Xt**, **Mt**, **XMt** and **NDH**, respectively. The temporary two data sets above are located on separate worksheets, named **rnahhhbase** (an Origin created baseline) and **RnahhhRAW** (the experimental data). The temporary data sets are indices created by Origin and do not have a worksheet created.

To open the Rnahhh worksheet

*Shortcut to worksheet:
Right-click on the data
trace and select **Open
Worksheet**.*

Select the **Plot...** command from the **Format** menu.
The **Plot Details** dialog box opens for the **rnahhh_ndh** data plot (if the **DeltaH** window is active).



- Click on the **Worksheet** button.
The **Rnahhh** worksheet opens.

Please note: If a worksheet cell is not wide enough to display the entire number, Origin will fill the cell with ##### signs. The full number is used by Origin. If you wish to view the full number you may increase the column width, by placing the cursor on the left or right border of the column name, waiting till the cursor changes to a double headed arrow, then moving the column edge to the left or right to increase the column width. Alternatively you may right-click the column name select properties from the drop-down list and increase the value in the **Column Width** text box.

	DH	INJV	Xt	Mt	XMt	NDH
	M	M	M	M	M	M
1	-1119.84952	4	0	0.651	0.09681	-13230.73628
2	-1111.34827	4	0.06284	0.64907	0.19391	-13130.29615
3	-1097.55602	4	0.12548	0.64714	0.29129	-12967.3443
4	-1077.75683	4	0.18795	0.64522	0.38896	-12733.42189
5	-1067.52519	4	0.25022	0.6433	0.48692	-12612.53766
6	-1037.99499	4	0.31231	0.64139	0.58517	-12263.64587
7	-1000.50813	4	0.37421	0.63949	0.6837	-11820.74826
8	-923.83212	4	0.43592	0.63759	0.78252	-10914.84072
9	-825.14833	4	0.49745	0.63569	0.88163	-9748.91693
10	-670.58561	4	0.55878	0.63381	0.98103	-7922.79781
11	-508.97161	4	0.61994	0.63192	1.08072	-6013.36964
12	-360.28215	4	0.6809	0.63005	1.18069	-4256.64162
13	-250.8639	4	0.74168	0.62817	1.28095	-2963.89295

Copy and Paste Worksheet Data

Data can be copied from a worksheet to the clipboard, then pasted from the clipboard into another Origin worksheet, a plot window, or another Windows application. To copy and paste worksheet data:

Select a range of worksheet values

- Select the initial cell, row, or column in the range.
To select a cell, click on the cell. To select an entire row, click on the row number. To select an entire column, click on the column heading.
- To select a contiguous portion of worksheet values, click on the first cell, row or column, keep the mouse button depressed, drag to the final cell, row, or column that you want to include in the selection range, then release the mouse button. The entire selection range will now be highlighted. (Note: If you ever wish to select a range of cells where the initial cell but not the final cell is in view, then click on the first cell and scroll to the final cell, press and hold the shift key then click the final cell.

Copy the selected values to the clipboard

- Choose **Copy** from the **Edit** menu, alternatively you may click the right mouse button inside the highlighted text and select Copy from the menu.
The selected values are copied to Windows clipboard.

Select a destination for the copied values



Shortcut:
To open a new worksheet click on the New Worksheet button from the Standard toolbar.

- To paste into a plot window, click on the plot window to make it active.
- To paste into a worksheet, click on the worksheet (or select **File:New:Worksheet** to open a new worksheet), then click to select a single cell. This cell will be in the upper left corner of the destination range.

- To paste into another Windows application, switch to the target application, then follow the pasting procedure for that application.
(*Shortcut:* If an application is already open you may switch to it by pressing and holding down the Alt key then pressing the Tab key till the application's icon is selected.

Paste the copied values from the clipboard to the destination

- Select **Paste** from the **Edit** menu, alternatively click the right mouse button and select Paste.
The selected values are pasted from the clipboard.

Note: It may happen that your worksheet does not show the data, but only displays pound signs, as shown on the right. The data is available for manipulations but is not displayed because the column is not wide enough. You may increase the column width by moving the cursor to the right edge of the column header (the cursor will change into a double headed arrow) then clicking and dragging the cursor to the right or you may right click the column heading, select properties, then increase the number for the column width.

	A[X]	B[Y]
1	0.09681	#####
2	0.19391	#####
3	0.29129	-12967.3443
4	0.38896	#####
5	0.48692	#####
6	0.58517	#####
7	0.6837	#####
8	0.78252	#####
9	0.88163	-9748.91693
10	0.98103	-7922.79781
11	1.08072	-6013.36964
12	1.18069	-4256.64162

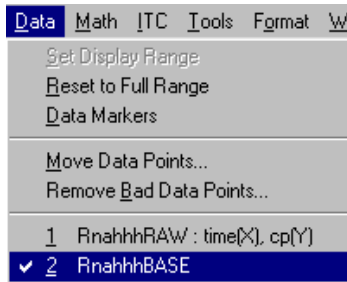
Exporting Worksheet Data

The contents of any worksheet can be saved into an **ASCII** file. In this section you will open the worksheet for the **RnahhhBASE** baseline data plotted in the **RawITC** window, and export the X and Y data to an **ASCII** file.

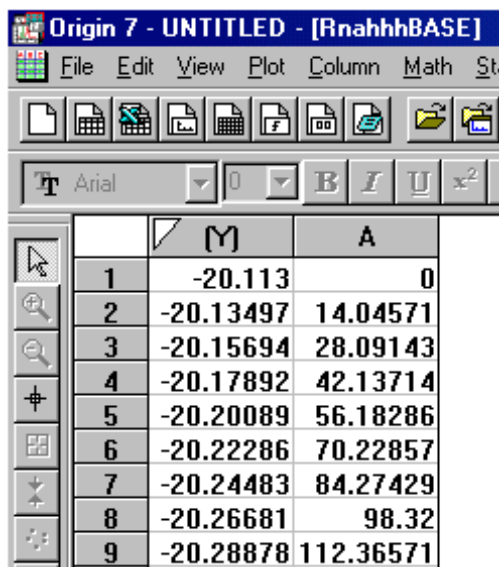
To open the Rnahhhbase worksheet

- Click on the **RawITC** window (or choose **RawITC** from the **Window** menu) to make it the active window.
- Select **RnahhhBASE** from the **Data** menu.
RnahhhBASE becomes checkmarked to show it is selected.

*Shortcut to worksheet:
Right-click on the data trace and select Open Worksheet.*



- Select **Plot...** from the **Format** menu.
The **Plot Details** dialog box opens.
- Click on the **Worksheet** button.
The **RnahhhBASE** worksheet opens.



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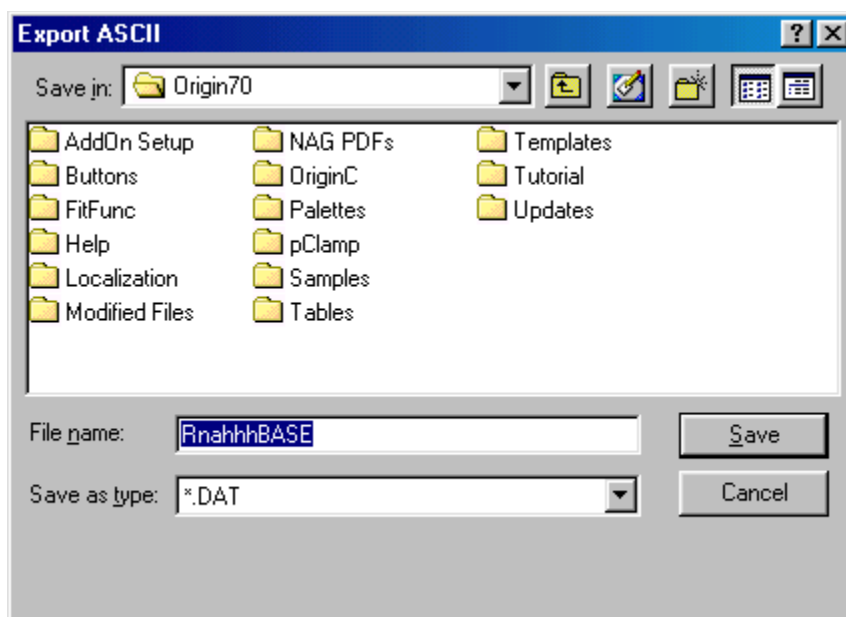
	M	A
1	-20.113	0
2	-20.13497	14.04571
3	-20.15694	28.09143
4	-20.17892	42.13714
5	-20.20089	56.18286
6	-20.22286	70.22857
7	-20.24483	84.27429
8	-20.26681	98.32
9	-20.28878	112.36571

To export the worksheet data as an ASCII file

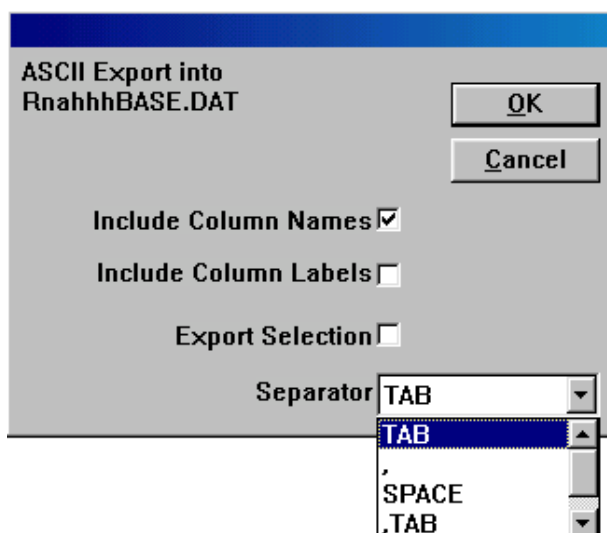
Shortcut:

*Right-click on the upper left containing white-space then select **Export ASCII**.*

- Select **Export ASCII...** from the **File** menu. The **Export ASCII** dialog box opens, with **RnahhhBASE.DAT** selected as the file name.



- Click **Save**.
- After you click Save in the Export ASCII dialog box, the ASCII Export Into dialog box opens.



- You may format the output of this ASCII file (Please refer to the Origin User's Manual for more information about Exporting worksheet data). This file may then be opened into any application that recognizes ASCII text files.

Importing Worksheet Data

ASCII files can be imported directly into an Origin worksheet or plot window. The basic worksheet Origin menu supports a number of additional file formats for importing data (Lotus, Excel, dBASE, LabTech, etc.) while the menus for ITC or DSC Data Analysis support routine ASCII import.

To import an ASCII file into a new worksheet

- Choose **Worksheet** from the **New** sub-menu under the **File** menu. A new Origin worksheet, **Data1**, opens.
- Select the **File : Import : ASCII** command. (If you like, you can select **File : ASCII : Options**. This will allow you to set ASCII file import options.) The **Import ASCII** dialog box opens, set to open a data file with a **.DAT** extension.
- Double-click on a file in the **File Name** list (for example, the **RnahhhBASE.DAT** file you just exported). The **RnahhhBASE** data imports into the worksheet.

To import an ASCII data file into a plot window



Shortcut:

*To create a graph, click on the **New Graph** button from the Standard toolbar*

- Choose **Graph** from the **New** sub-menu under the **File** menu.
- Choose **Import ASCII: Single File** from the **File** menu.
- Select the **rnahhhBASE.dat** ASCII file from the **Files** list. Enter the appropriate Initial X Value (0 for RnahhhBASE.dat) and Increment in X (28.25287) and click **OK**.