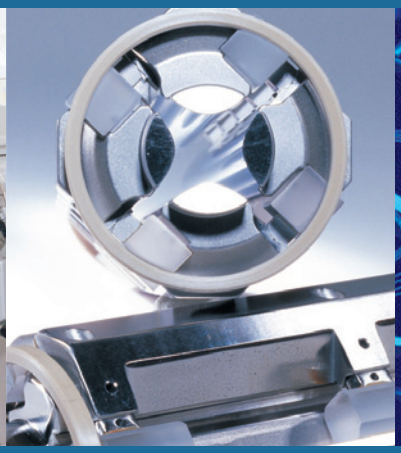
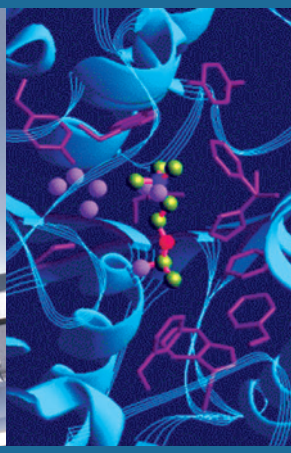
Thermo Fisher Scientific

Isodat 3.0

Simultaneous ASCII Data Export

Revision A - 1250500





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Isodat 3.0 - Simultaneous ASCII Data Export

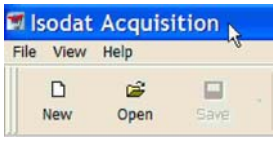
This manual describes how raw data are exported by Isodat 3.0 as ASCII data (in csv format) during any running Continuous Flow acquisition. Depending on the acquisition time of the individual acquisition, directories will be created for saving fractions of the exported data.

In addition to the common separate data export after a measurement in Isodat 3.0, this gives the user online access to results already before an acquisition is finished. Thereby, data interpretation and measures for process control depending on signal intensity are possible promptly.

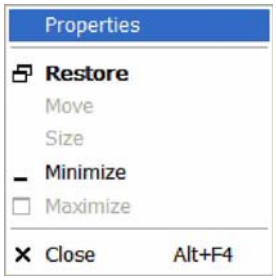
This manual deals with the following topics:

Activating Script Bar

Start Isodat Acquisition.



Right-click on the Isodat Acquisition title bar.



Choose **Properties**.

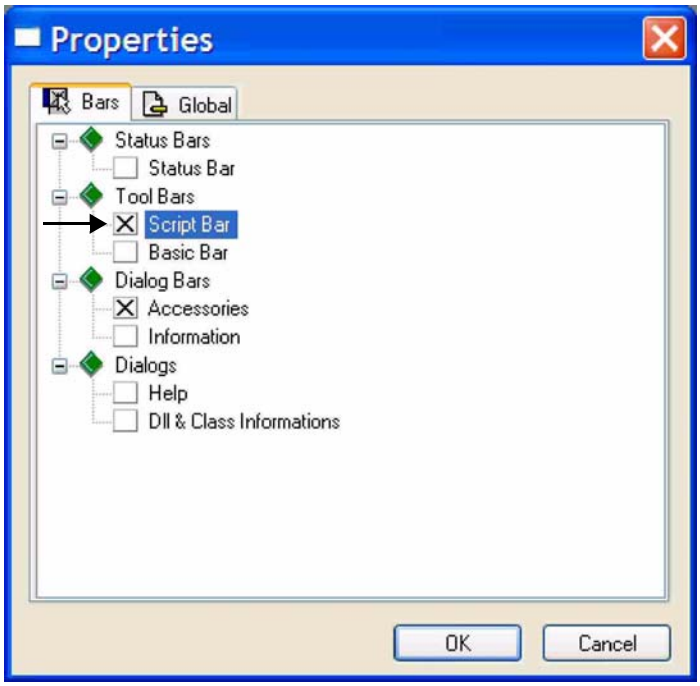


Figure 1. Marking Script Bar checkbox

Mark the **Script Bar** checkbox. See Figure 1.

The script bar will appear. Move the script bar until it is arranged in a row with the other bars.

Enabling Snapshot Script

Click on the **New** button.

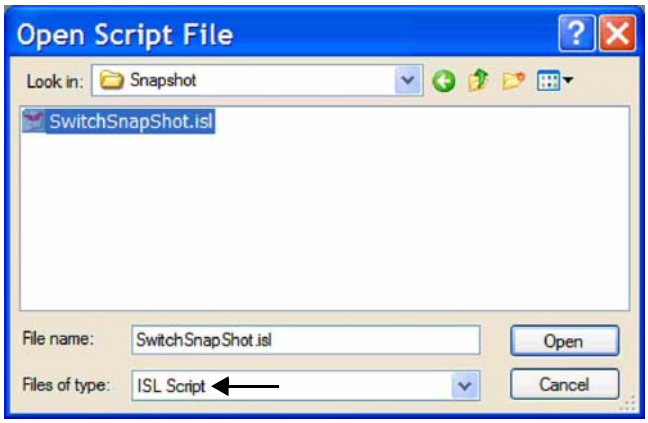


Figure 2. Selecting snapshot script

Browse to the directory \Thermo\Isodat NT\Global\ISL\Snapshot. At Files of Type select **ISL Script**. See Figure 2.

Double-click on the snapshot script **SwitchSnapShot.isl**. A new button, SwitchSnapShot, appears at the script bar.

To enable the snapshot script, click on the **SwitchSnapShot** button.

Confirm with **OK**.

Figure 3. Close all open chromatograms

Close all open chromatograms, especially the measurement file acquired at least. See Figure 3.

Accessing Result Files

1. Start a sequence.

2. In the File Browser, select the **Results** tab.

   The results folder ACQ-Results will be shown. See Figure 4.

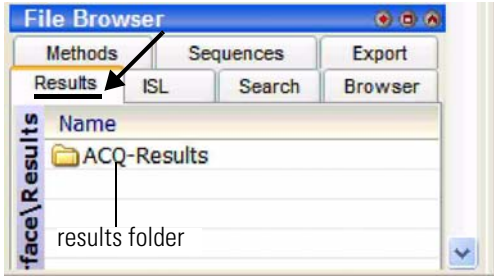
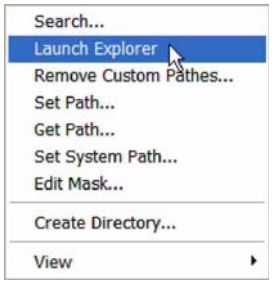


Figure 4. Selecting Results tab of File Browser

3. Right-click into the grid of the File Browser and select **Launch Explorer**.



As usual, the folder ACQ-Results contains chromatograms as dxf files. Their number equals the number of sequence lines you previously specified during sequence creation. Additionally however, a subfolder SnapShot has just been created. See Figure 5.

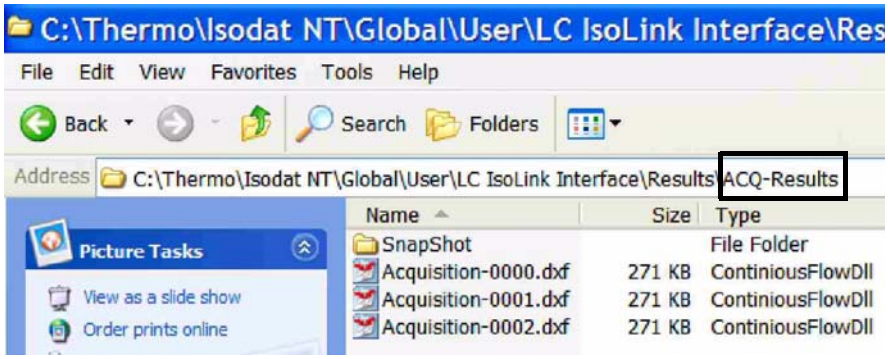


Figure 5. Contents of folder ACQ-Results

For any of the acquisitions, a corresponding subfolder with the same name will be created in SnapShot.

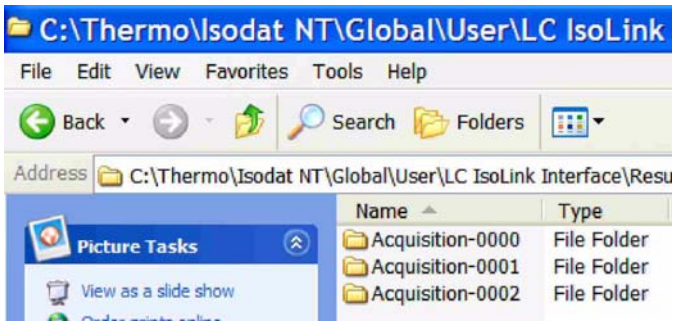


Figure 6. Contents of subfolder SnapShot

See Figure 6 as an example with three folders (Acquisition-0001, Acquisition-0002 and Acquisition-0003).

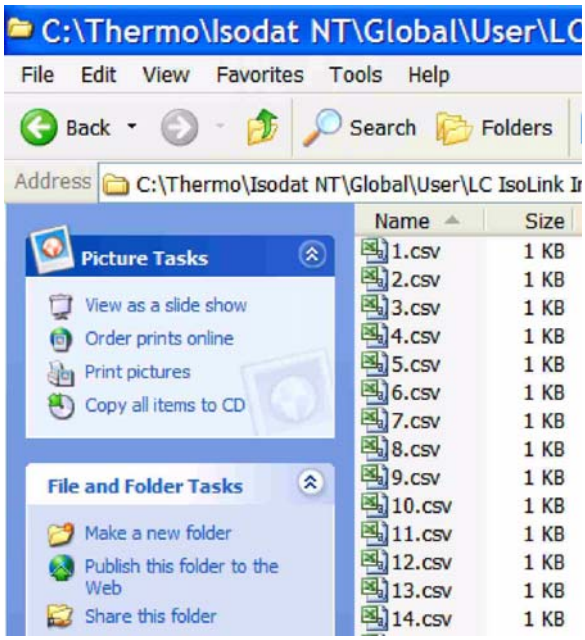


Figure 7. Contents of one subfolder Acquisition-000k

Each of these folders contains measured result files in csv format, that is as comma-separated values. The csv files are named 1.csv, 2.csv, etc. Long measurements will lead to more csv files than short ones. See Figure 7.

Within each acquisition folder numbering starts anew with 1.csv, 2.csv, etc.. The individual export files (*.csv) can now be examined one after another in another program, for example a spreadsheet, while the measurement is still running.

Structure of a Single Result File

All csv-files have the same structure. Figure 8 shows it for an arbitrary csv file.

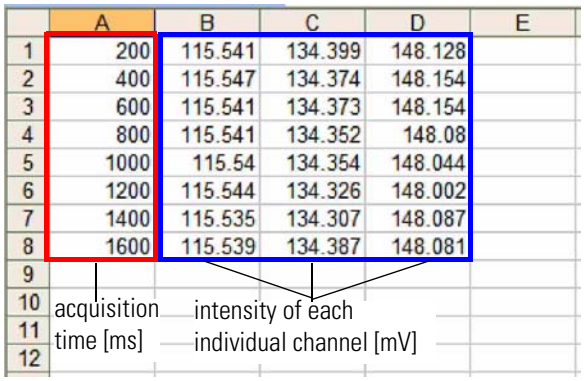


Figure 8. Structure of a result file

The leftmost column A lists the acquisition times in ms. They are given in steps of ascending order which reflect the selected integration time.

Each of the following n columns (that is B, C, D,...) represents the intensities one of the n measured channels. As an example, three measured channels (m/z 44, m/z 45 and m/z 46) will lead to three columns.

Usually, a csv file comprises eight lines. In seldom cases however, it may contain more or less than eight lines. According to the default settings previously adjusted in Isodat Configurator, each intensity value is given with three decimal places.

Note Isodat will not delete any of the generated csv files. Delete the csv files you do not need anymore on your own. ▲

To disable the snapshot script, click on the **SwitchSnapShot** button.

Confirm with **OK**.

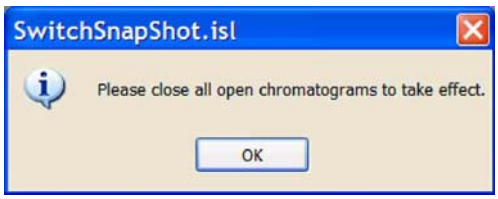


Figure 9. Close all open chromatograms

Close all open chromatograms. See Figure 9. Creation of further csv files will be stopped.

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