GSpectrum manual

Feedback

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	TITLE : GSpectrum manual		
ACTION	*NAME*	*DATE*	*SIGNATURE*
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REVISION HISTORY			

NUMBER	DATE	DESCRIPTION	NAME
GSpectrum Manual V0.3	August 2012	Jean Bréfort jean.brefort@normalesup.org GNOME Documentation Project	
GSpectrum Manual V0.2	April 2010	Jean Bréfort jean.brefort@normalesup.org GNOME Documentation Project	
GSpectrum Manual V0.1	October 2008	Jean Bréfort jean.brefort@normalesup.org GNOME Documentation Project	

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Abstract

GSpectrum is a simple spectrum viewer.

Introduction

The GSpectrum application is a spectrum viewer. It can load a variety of files in the JCAMP-DX format. It can also load NMR data from the NUTS format.

Supported spectra include UV-visible, IR, Raman, NMR (both spectra and FIDs), and Mass.

Chapter 1

Getting started

1.1   To Start GSpectrum

You can start GSpectrum in the following ways:

Applications list Choose "Spectrum viewer". It might be listed either in the Education or Science category.

Command line Type **gspectrum**, then press **Return**.

1.2   When You Start GSpectrum

When you start GSpectrum, the following window is displayed:
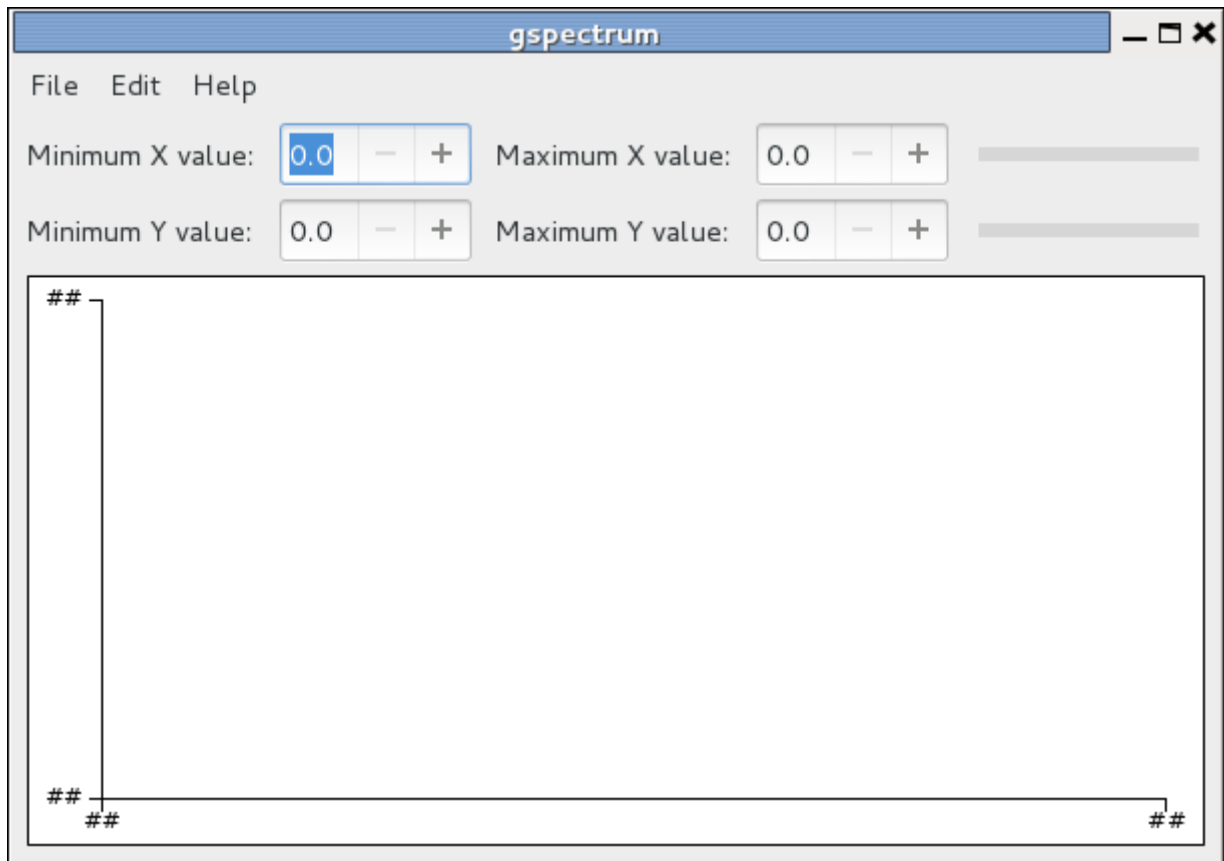
Figure 1.1: GSpectrum document window

The GSpectrum window contains the following elements:

Menubar The menus on the menubar contain all of the commands you need to work with files in GSpectrum.

Display area The display area contains the contents of the file that you are displaying and/or editing.

1.3   To Open a File

To open a file, choose File → Open to display the Open File dialog. Select the file that you want to open, then click OK. The file is displayed in a new GSpectrum document window.

To Open a recently opened file, choose the appropriate entry in File → Open recent

GSpectrum can open files on a remote server.

You can open multiple files in GSpectrum. Each file is opened in it's own top-level window.

1.4   To Open Multiple Files from a Command Line

You can run GSpectrum from a command line and open a single file or multiple files. To open multiple files from a command line, type the following command, then press **Return**:

gspectrum *file1 file2 file2 ...*

where file1 and others, might be relative, absolute paths or URIs.

When the application starts, a GSpectrum window is created for each file that you specified.

Chapter 2

Usage

2.1 To Customize the spectrum view

The customization options depend on the spectrum type.

When a spectrum is opened in a new window, the displayed data are those directly read from the file. The abscissa axis might be inverted in some cases, according to current usage.

In the simplest case, the toolbar looks like:
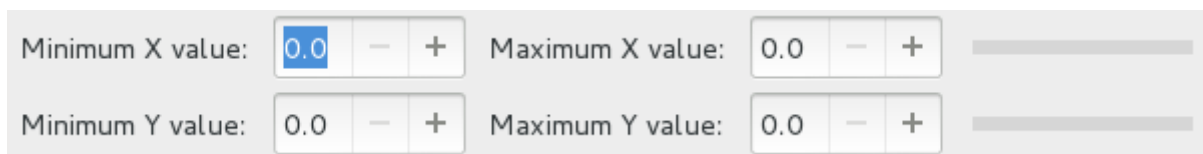
Figure 2.1: GSpectrum default toolbar

You can set the values of the minimum and maximum displayed coordinates for both axes. These limiting values are constrained to be within the actual data intervals.

When only a part of the spectrum is displayed, the appropriate slider can be used to scroll through the spectrum view. The spectrum moves in the same direction as the horizontal slider and to the top when the Y axis slider is moved to the right.

When the spectrum is a UV-Visible spectrum, additional controls are available:

Figure 2.2: toolbar for UV-visible spectra

The abscissa can be switched between wavelength in nanometers and wave number in cm^{-1} and the axis inverted (high values at left) or not, and the ordinate can be either absorbance or transmittance.

The toolbar is almost identical for IR spectra. The only difference is that wavelengths are in micrometers instead of nanometers:

Figure 2.3: toolbar for IR and Raman spectra

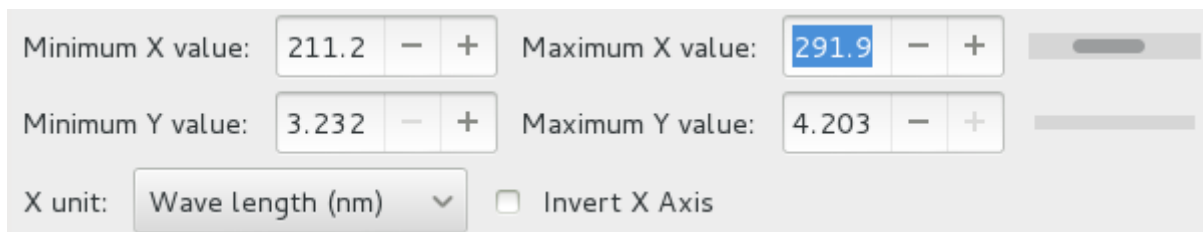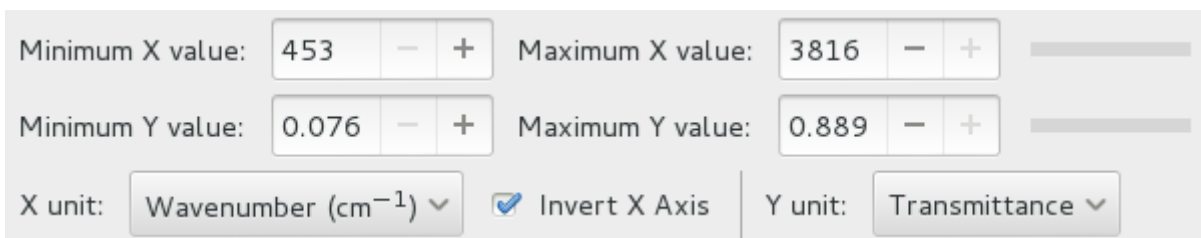The abscissa units available for NMR spectra are ppm and Hz. The integration curve can also been displayed or hidden:
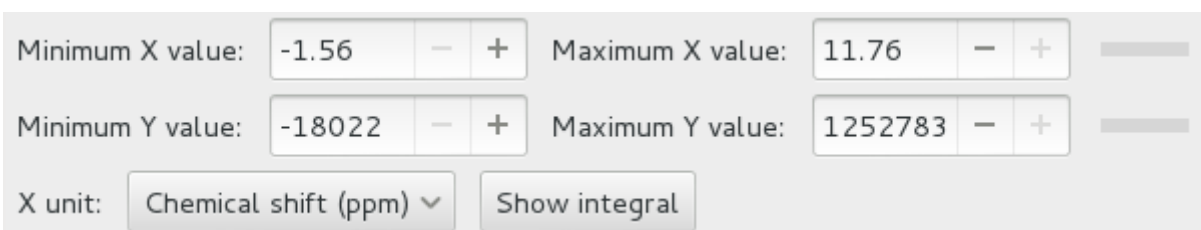

Figure 2.4: toolbar for NMR spectra

An NMR FID can be transformed to the spectrum unless some parameters are missing in the source file:
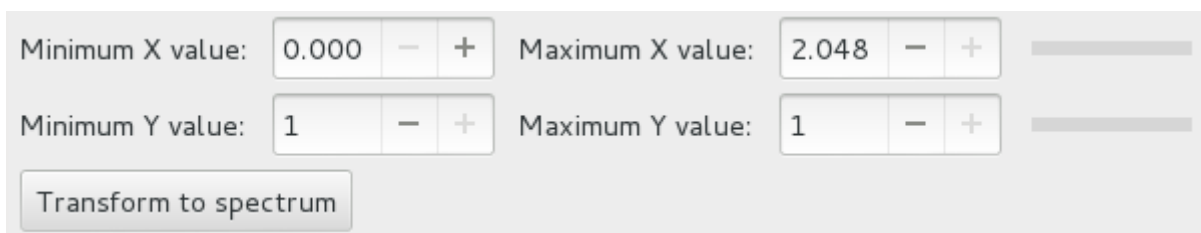
Figure 2.5: toolbar for NMR FID

2.2   Export the Spectrum as an Image

To export the displayed spectrum to an image, use File → Save As Image.

Available formats are SVG, EPS, PS, PDF, and formats that support writing in GdkPixbuf.

To choose a format, you can use an appropriate file name extension, or explicitly select a format in the combo box. With the first method, if GSpectrum does not recognize an extension, the exported file will be a SVG file. GSpectrum will add an extension to the file name if needed.

You might change the default width and height of the exported image using the appropriate entries.

Postscript and PDF files can also be produced using the FilePrint... command.

2.3   To Print the Spectrum

To print a spectrum, choose File → Print....

File → Preview opens a window with a preview of the printed output.

To tune the printed output, chooseFile → Page setup... as explained below.

2.3.1 The page setup dialog.

The first tab of the dialog concerns the paper and margins setup. Headers and footers are not supported in the version of GSpectrum
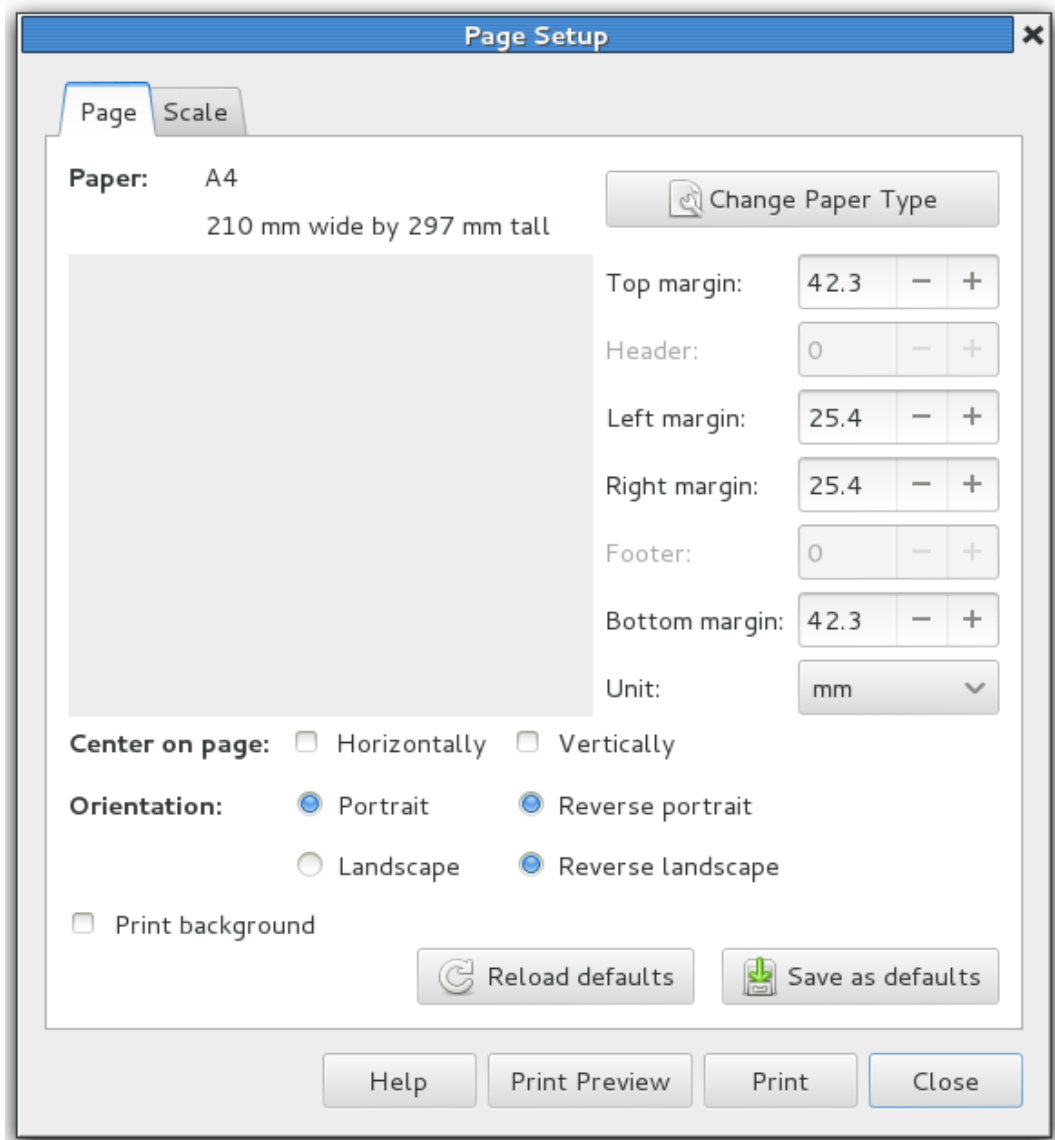
Figure 2.6: The Page Setup tab.

The second tab allows you to choose the scale of the output. With no scaling or scaling at 100%, the output will have the same size in points as the size in pixels on the screen. If you choose automatic scaling, you can make the output fill the available space either horizontally, vertically, or both (unchecking both options is equivalent to no scaling).

Printing to more than one page is not supported in this version of GSpectrum

Figure 2.7: The Print Scale tab.

Chapter 3

Support.

3.1   To Ask a Question

If you choose Help → Ask a question, your mail client should pop up with a new message to the Gnome Chemistry Utils mailing list.
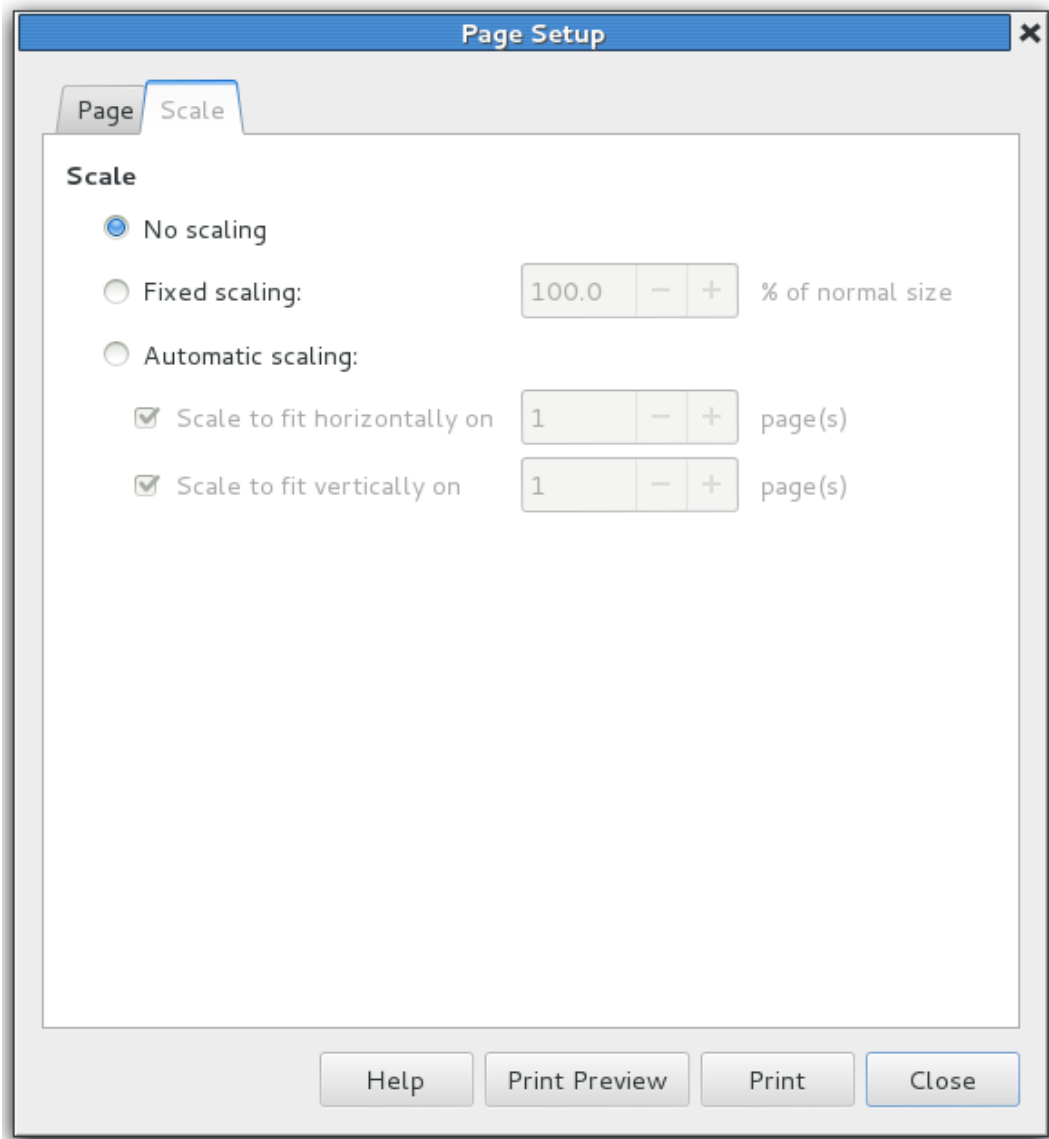
Another way to get some help is to connect on the #gchemutils IRC channel on the irc.gimp.net network and ask your question there (if you are not alone on the channel).

3.2   To Find the Gnome Chemistry Utils on the Web.

If you choose Help → Gnome Chemistry Utils on the web, the default web browser should pop up and display the main page for the Gnome Chemsitry Utils.

The main page is http://gchemutils.nongnu.org and the project page at Savannah http://savannah.nongnu.org/projects/gchemutils.

3.3   To Report a Bug

To report a bug, you must use the bug page for the Gnome Chemistry Utils at Savannah. You can access it by choosing Help → Report Bugs (hopefully you'll have only one at a time to report).

You can also use a web browser to go to the bug report page address directly. The bug repository is at https://savannah.nongnu.org/-bugs/?group=gchemutils

Chapter 4

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