



## Mnova for metabonomics

### MestReNova: NMR plugin

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## Introduction

Mnova allows you to easily process large datasets with the best quality in order to obtain the most precise results. Once datasets have grown to 20-200 spectra, **manual processing is no longer an option**.

Mnova can automate the processing of **large datasets of biofluids** to extract an ASCII file ready for the statistical measurement.

Mnova includes powerful specific **Phase and Baseline Correction algorithms for 1D and 2D biofluid spectra** in order to get the correct quantification

## Getting Started

Mnova can be used on large datasets of biofluid spectra in two main ways, depending on the size of the dataset.

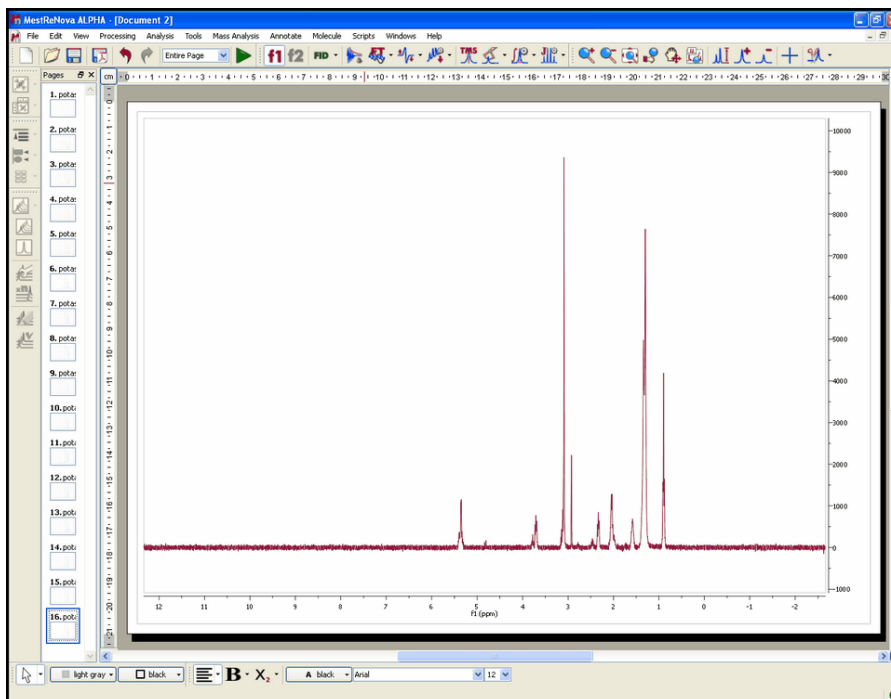
**Graphical (<100 spectra):** this mode allows all processing commands to be executed on a group of spectra simultaneously making possible the interaction with all spectra at the same time.


**Scripting (>100 spectra):** the user will only need to open a single spectrum of the dataset and optimize the processing in order to apply it to the remaining spectra by using the scripting capability implemented in Mnova.

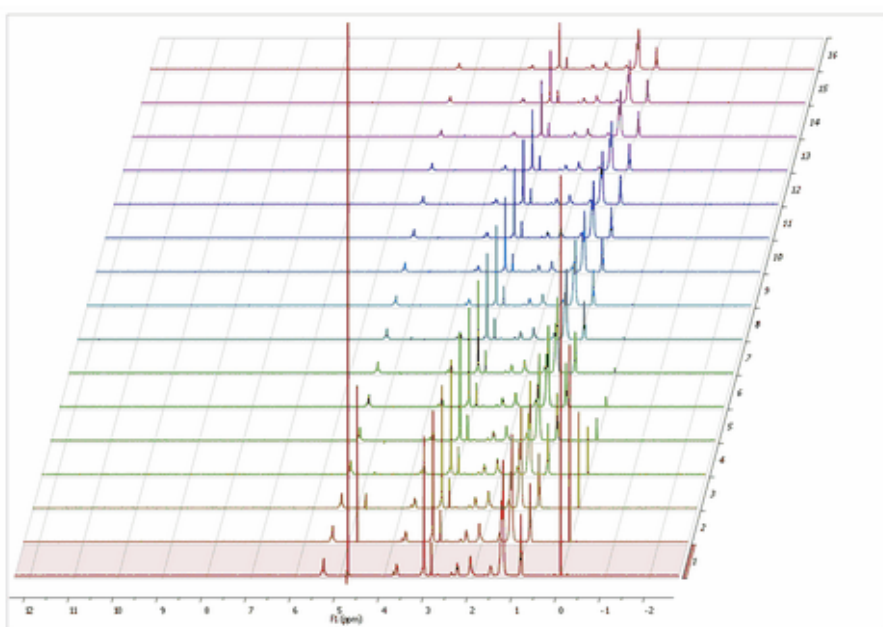
## Processing Basics

Let's take a look at the '**graphical method**'.

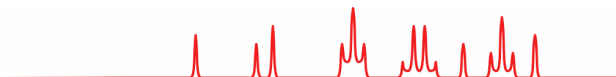
1. When the dataset is small, we can drag the spectra folders to Mnova in order to get all the spectra fully processed. In this case I have dragged 16 spectra folders to the Mnova icon. After about 5 seconds, I got all the spectra fully processed as you can see in the picture below



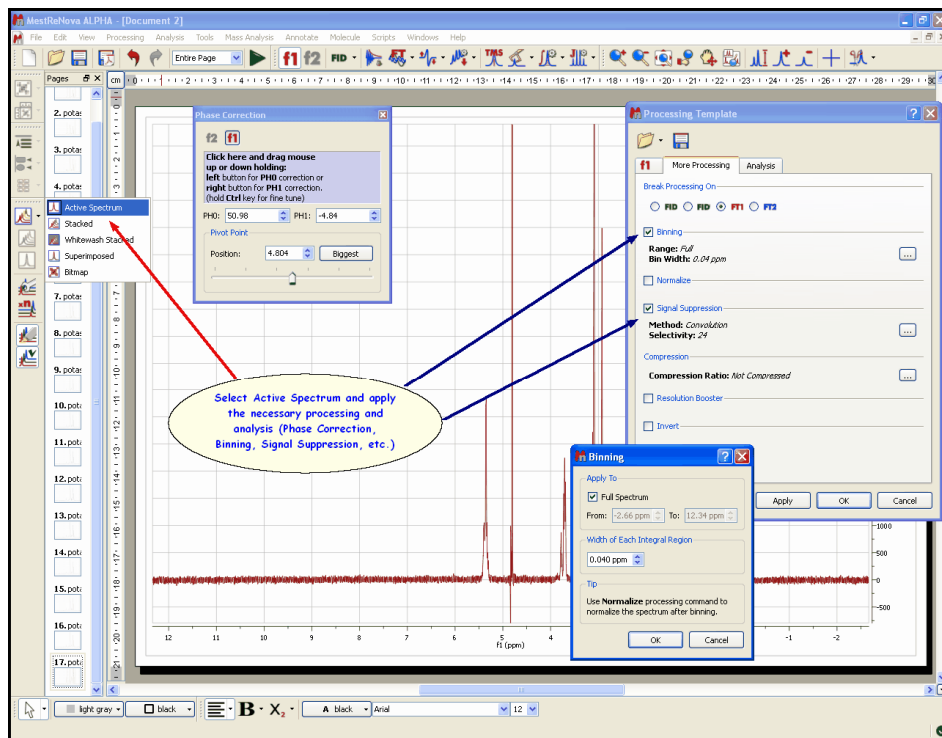
2. Select all the spectra in the page navigator in order to create the stacked spectra. We can do it by pressing 'Ctrl+A' or by following the menu 'Edit/Select All' and then clicking on the 'Stack Spectra' button  (in the left-vertical toolbar) or going to the 'Tools/Stack Spectra' menu.



3. Select one of them (by selecting 'Active Spectrum' in the Stack scroll down menu of the left-vertical button) and apply the necessary processing and analysis (phase and baseline

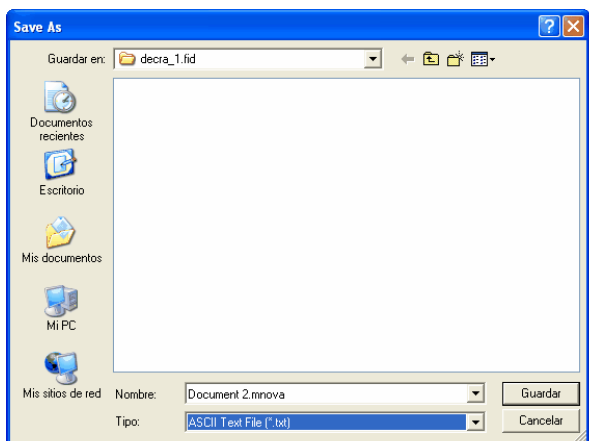


corrections, binning, signal suppression...). The operations to the first spectrum will be applied simultaneously over the whole dataset.



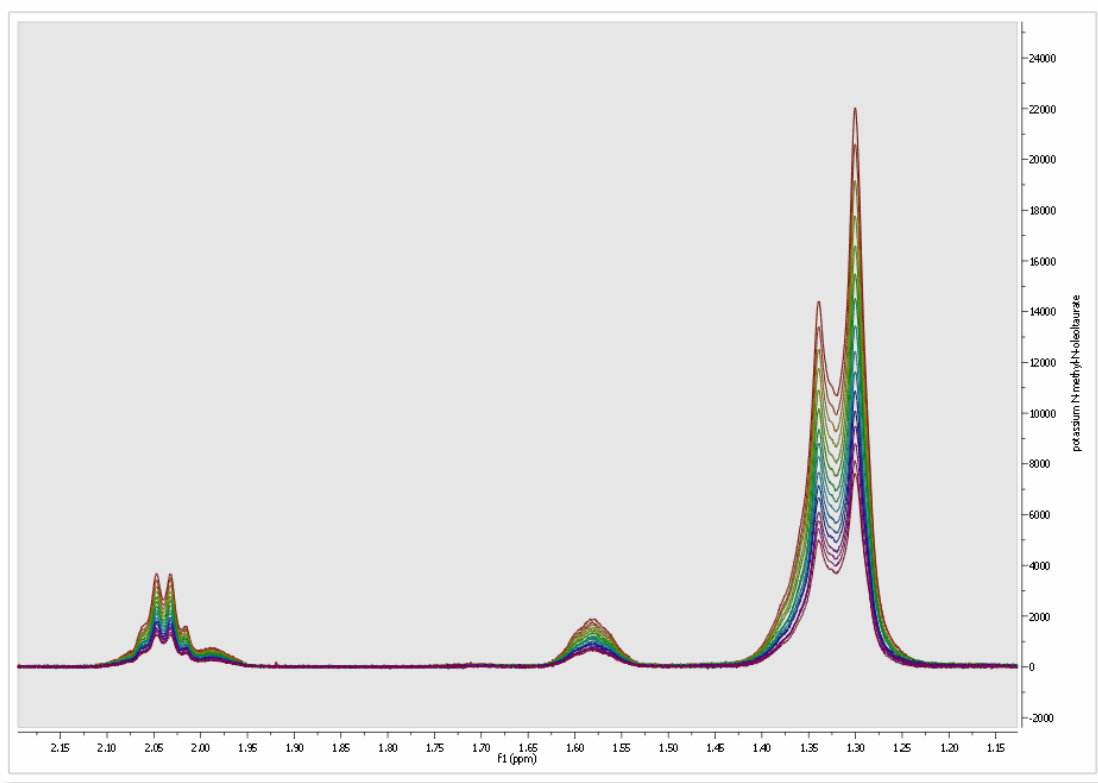
Mnova incorporates several specific features for biofluid samples; such as **Automatic Phase and Baseline corrections algorithms**, **Solvent Suppression** (to remove, for example, the dispersive signal of the water), **Auto-tuning referencing**, **Binning** (or bucketing), **Global Spectral Deconvolution** (work in progress).

4. Once the processing and analysis have been made, we can export to an ASCII file for the PCA or PLS, just by following the menu 'File/Save As/ASCII text file (\*.txt)'.





It will be possible to superimpose all the spectra to double check for example that all spectra are perfectly aligned or referenced. To do that, just highlight the stacked spectra and go to the menu 'Tools/Superimpose Spectra':



## Scripting Method

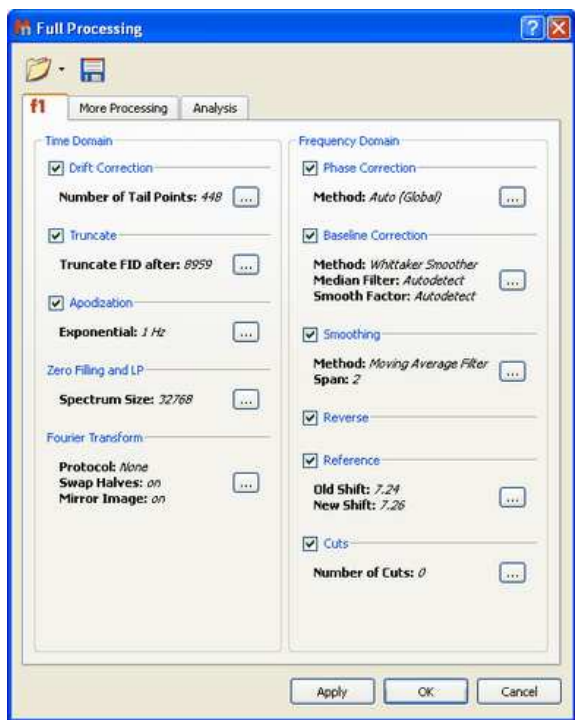
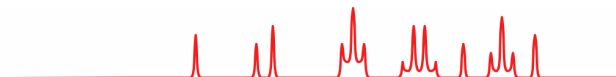
Let's take a look at the '[Scripting method](#)'.

Mnova includes **Scripting capabilities** to automate the previous process with the ability to create Processing Templates which can be used with our Script engine to perform batch processing.

**Mnova** includes a powerful and flexible feature which allows the user to easily automate the full processing of both 1D & 2D NMR data sets. This is ideal for the batch processing of spectra of the same type, and can also incorporate analysis operations.

For example, let's say you have acquired 20 proton spectra which you want to process using the same processing operations. The procedure is very simple:

1. Load one spectrum and process it as desired.
2. Go to **Process/Full Processing**. The following dialog appears:

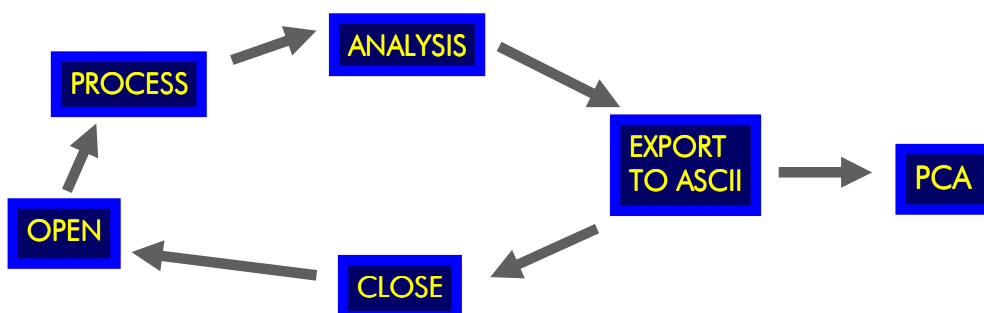


This dialog includes all the processing and analysis features implemented in **Mnova**. You can choose the required options by selecting the check boxes and, if necessary, specify options by clicking the button next to the corresponding command.

3. Once you are happy with the result, **save** the script file to a Mnova Processing file (\*.mnp) by clicking on the save button in the dialog box.

Once you have saved this template, you will be able to run a script to process all the spectra in the same way.

If the number of datasets is too large, Mnova is able to open, process (apodization, FT, Zero Filling, LP, phase and baseline Correction...), analyze (binning, etc.), save to an ASCII file and close the spectrum, in order to open the next one and continue with the processing (to avoid an excessive use of memory). If the number is not large, Mnova can keep all the spectra fully processed on screen.

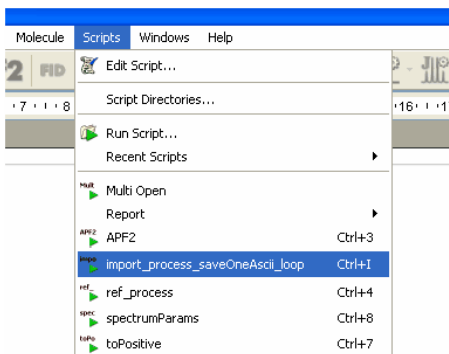




You can use the below script to automate the above process and save all the result into the same ASCII file. You will be able to download it from this link:

<http://www.mestrec.com/recursos.php?idr=121&i18n=1>

Copy this script to the scripts folder of Mnova, restart the software and the script will appear under the 'Scripts' menu.



Please bear in mind that you can introduce this script into the toolbar by using the 'Toolbar Customization' feature (View/Toolbars/Customize Toolbars).

To read more about Mnova scripting, please download this tutorial:

<http://www.mestrec.com/recursos.php?idr=112&i18n=1>

```
//<GUI menuname="import_process_saveOneAscii_loop"shortcut="Ctrl+I"tooltip="Auto Process
and Save as ASCII"/>
/*****
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This file is part of the MNova scripting toolkit. Authorized users of MNova Software may
use this file freely, but this file is provided AS IS with NO WARRANTY OF ANY KIND,
INCLUDING THE WARRANTY OF DESIGN, MERCHANTABILITY AND FITNESS FOR A PARTICULAR PURPOSE.
*****/
// This example function demonstrates how to apply some processing to a set of spectral
files and to save the result in a single ASCII file.
function import_process_saveOneAscii_loop()
{
    const procName = "c:/procTemplates/proc.mnp"; // Processing file. It must be
created in the Processing Template dialog of MestReNova.
    const fileMask = "fid"; // This mask specifies files to be processed.
    const dirMask = "*"; // This mask specifies directories to be scanned for spectra.

    // Select a directory with spectral data
    const specDirKey = "import_process_saveOneAscii_loop/SpectraDir";
    var dirName = FileDialog.getExistingDirectory(settings.value(specDirKey,
Dir.home()), "Select Spectra Directory");
    if (!dirName)
        return;
    var dir = new Dir(dirName);
    dir.cdUp();

    // Select a file to save the output
    const outDirKey = "import_process_saveOneAscii_loop/OutputDir";
    var saveDir = settings.value(outDirKey, Dir.home()); // Get last used directory
name
```



```

var fileName = FileDialog.getSaveFileName("ASCII Files (*.txt)", "Select Output
File", saveDir);
if (!fileName)
    return;

// Open the selected file and create a text stream mapped to it
var fout = new File(fileName);
settings.setValue(outDirKey, fout.absDirPath); // Save the directory name to be
used another time the script is called
var sout = new TextStream(fout);
sout.precision = 10;

// Temporary file name
const lastOutName = Dir.temp() + "/import_process_saveOneAscii_loop.lastOut.tmp";
if (File.exists(lastOutName))
    File.remove(lastOutName);

// The below function getMaskFiles is located in the files.qs script.
var files = getMaskFiles(dirName, dir.absPath, fileMask, dirMask, true);
for(var fi = 0, length = files.length; fi < length; fi++)
{
    var dw = new DocumentWindow(Application.mainWindow.newWindow()); // Create
new document window
    if (serialization.open(files[fi]))
    {
        nmr.process(procName); // Apply processing template
        var spec = new NMRspectrum(nmr.activeSpectrum());

        fout.open(File.WriteOnly);

        var flastOut = new File(lastOutName);
        var slastOut = new TextStream(flastOut);
        if (!fi)
        {
            // Put fist column of the file in ppm. The scale is taken
from the first spectrum.
            flastOut.open(File.WriteOnly);
            slastOut.precision = 10;

            var ppm = spec.hz()/spec.frequency();
            var dPpm = spec.scaleWidth()/spec.count()/spec.frequency();
            for(var si = spec.count()-1; si >= 0; si--)
            {
                slastOut.write(ppm, "\n");
                ppm += dPpm;
            }
            flastOut.close();
        }
        flastOut.open(File.ReadOnly);

        for(var si = spec.count()-1; si >= 0; si--)
            sout.write(slastOut.readLine(), "\t\t", spec.real(si),
"\n");

        fout.close();
        flastOut.close();
        flastOut.remove();
        if (fi < length-1)
            File.copy(fileName, lastOutName);
    }
    dw.close(); // Close document window of processed spectrum
}
}

```