NMRViewer 1.0

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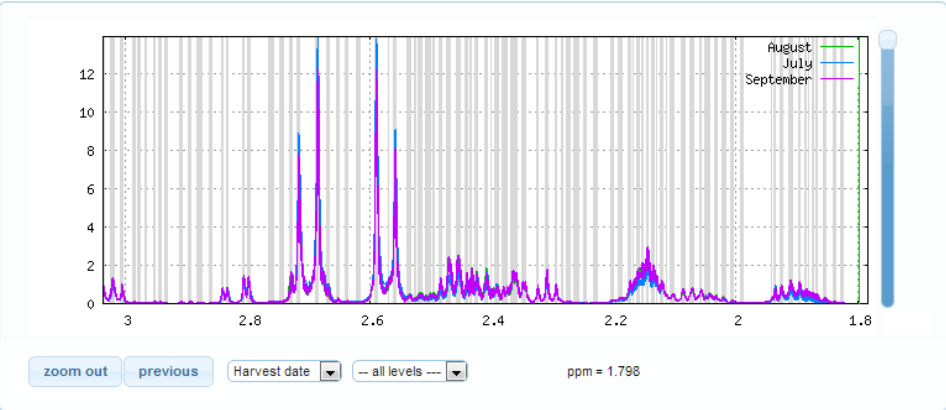
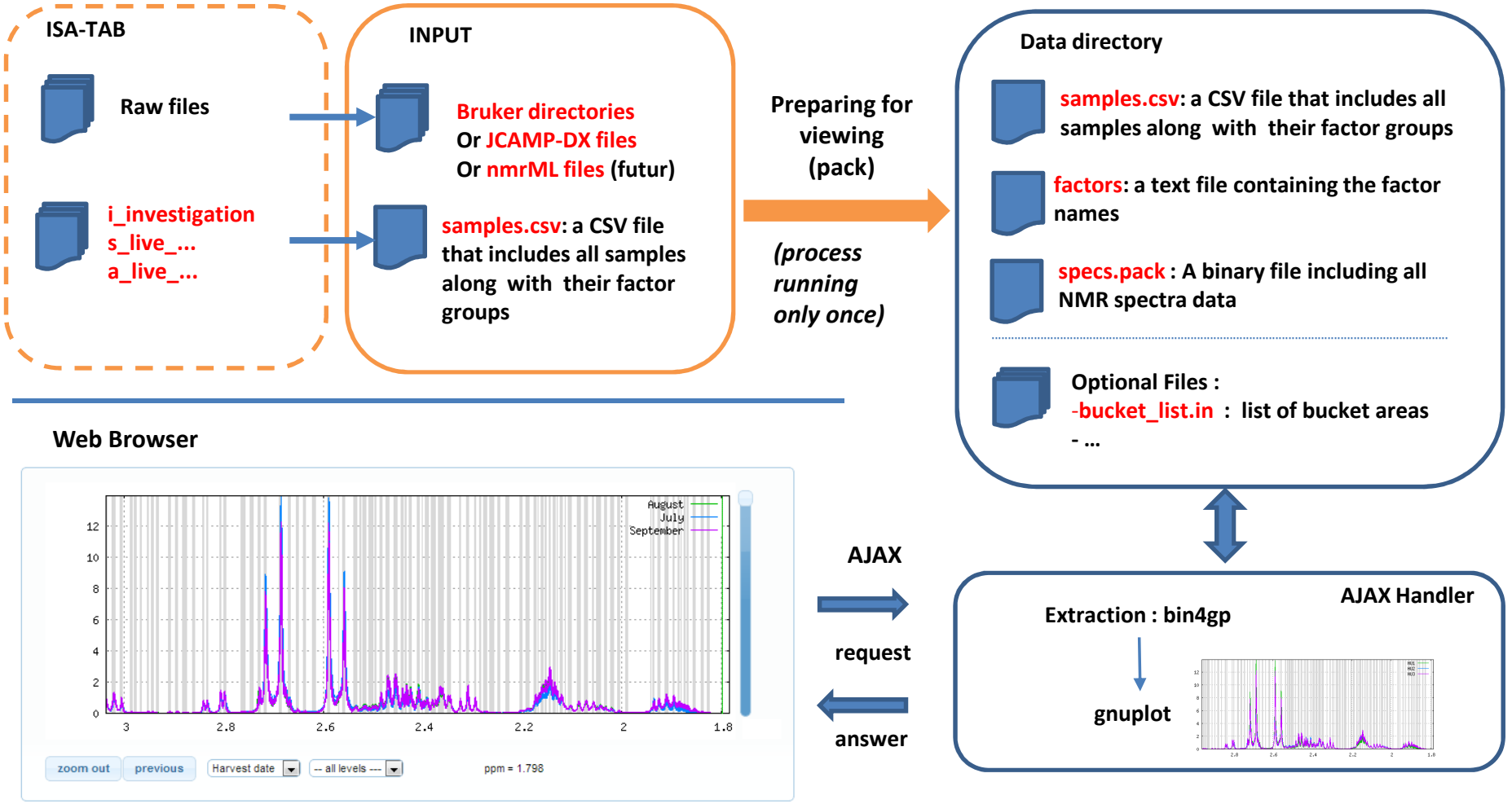
A Web Viewer for NMR spectra design-based on the jQuery framework



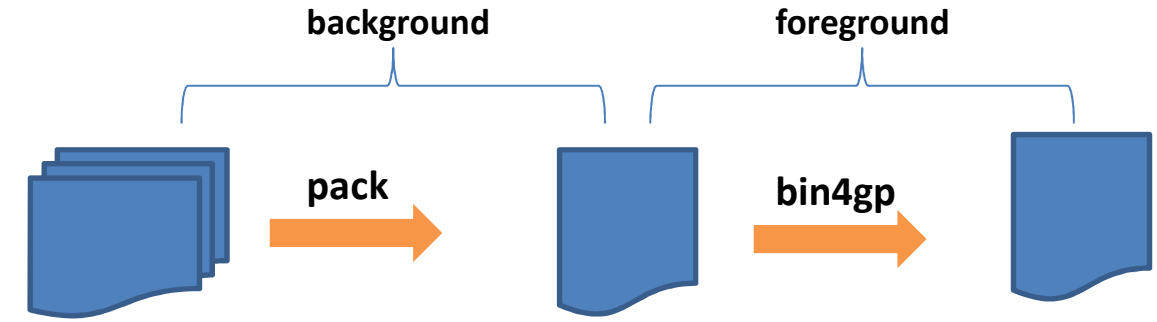
NMR spectra viewer : An overview of how it works



Web design based on the jQuery framework (client side) , PHP, C, gnuplot 4.3 (server side)

NMR spectra viewer : Why it runs so fast ?

Because **Text to Binary conversion is time consuming**, so we do not manipulate data as text format but **only as binary format in foreground process**.
Text to Binary conversion is set up in a background process, only once.



Bruker directories
Or JCAMP-DX files
Or nmrML files (futur)

specs.pack
A binary file including all NMR spectra data

specxx.bin
spectra intensity values within a ppm range

Gnuplot :
`plot 'specxx.bin' binary record=…`

NMR spectra viewer : How to process with an ISA-TAB archive ?

Step 1: unzip the isatab archive

```
unzip HUGO07.isa -d /tmp/HUGO07/
```

Step 2: Preparing for viewing (pack)

- ❑ Create an entry in your dataset repository

```
mkdir ./data/HUG07
```

- ❑ Convert isa_tab metadata files into a CSV file

```
nmrview/bin/tab2csv -d /tmp/HUGO07/ -o samples.csv –v
```

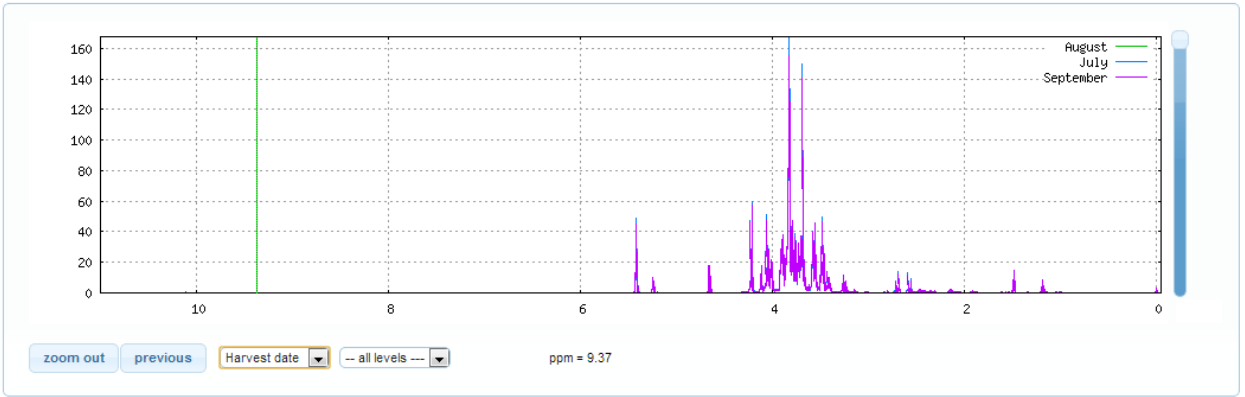
- ❑ Create the "pack" file

```
nmrview/bin/pack_bruker -i /tmp/HUGO07/samples.csv -o ./data/HUGO07/ -h
```

NMR spectra viewer : jQuery UI plugin

---------- simple.html ----------

```
<!DOCTYPE html PUBLIC "-//W3C//DTD XHTML 1.0 Strict//EN" "http://www.w3.org/TR/xhtml1/DTD/xhtml1-strict.dtd">
<html xmlns="http://www.w3.org/1999/xhtml" xml:lang="en" lang="en">
<head>
  <meta charset="utf-8" />
  <TITLE>NMR Viewer</TITLE>
  <link rel="stylesheet" href="/nmrview/css/redmond/jquery-ui.min.css">
  <script src="http://code.jquery.com/jquery-1.9.1.js"></script>
  <script src="http://code.jquery.com/ui/1.10.0/jquery-ui.js"></script>
  <script src="/nmrview/js/ui.nmrview.js"></script>
  <script>
  $(function() {
     $( "#nmrview" ).nmrview({
       url:'/nmrview/view',  dataset: 'HUGO07', colorby: 0, width: 'auto'
     }).show();
  });
  </script>
</head>
<body>
   <div id="nmrview"></div>
</body>
</html>
```



NMR spectra viewer : TODO

Annotation

❑ Need to design a simple mechanism to add annotations

❑ Annotations in a file with a format to be defined (text file or nmrML)

❑ Each area, typically defining a bucket or peak, would be highlighted by moving mouse over it (mouseover event) and the corresponding annotation text would be displayed into a configurable html element.

❑A use case could be based on a recent work (1) that aims to propose a list of putative compounds for clusters of buckets.

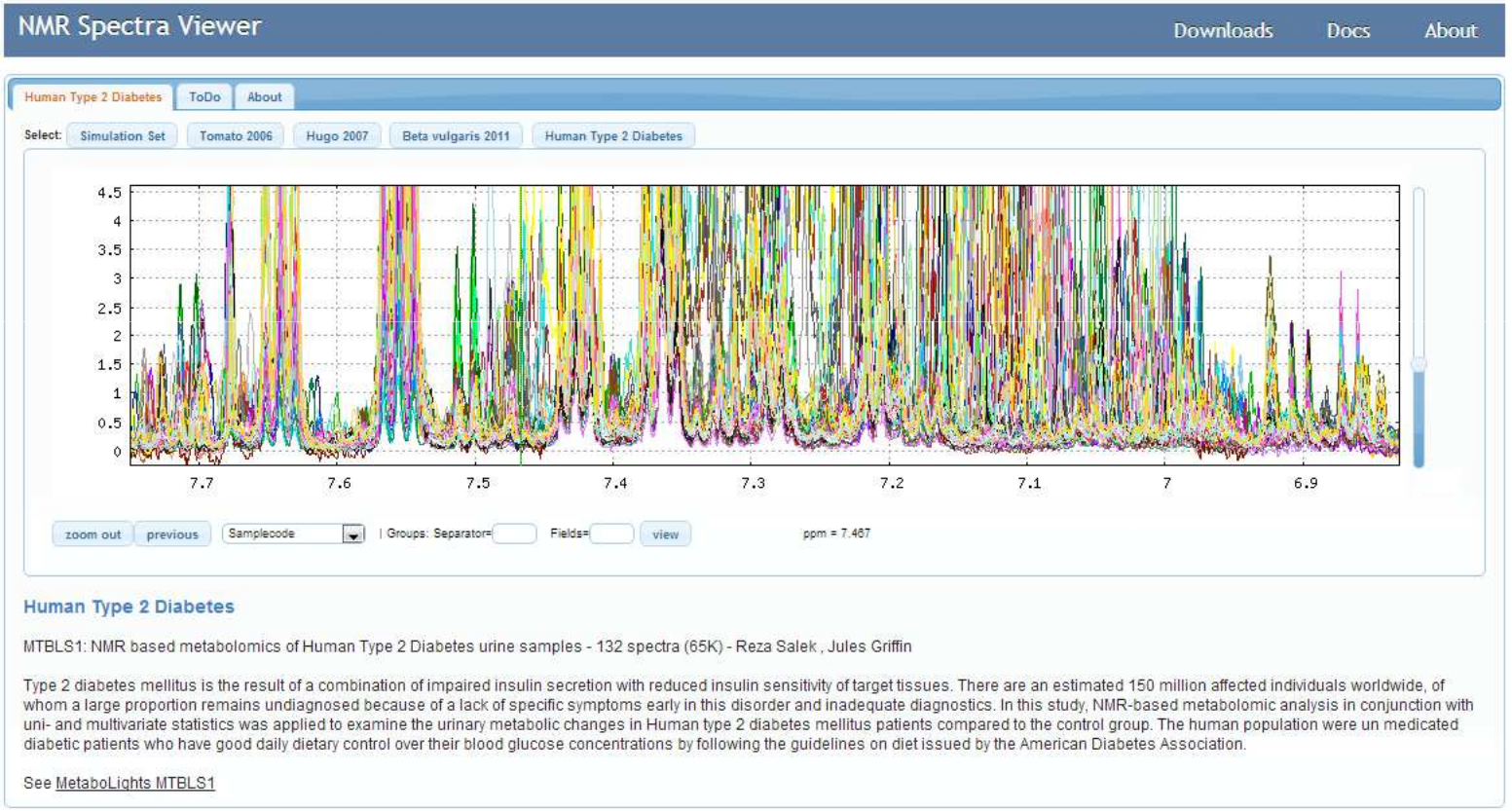
(1) Daniel Jacob, Catherine Deborde and Annick Moing (2013) An efficient spectra processing method for metabolite identification from 1H-NMR metabolomics data. Analytical and Bioanalytical Chemistry (doi:10.1007/s00216-013-6852-y)

CLUSTER ID=12
PPM: 2.536, 2.559, **2.589**, 2.665, 2.695
DBREF0010 (citric acid) : Score=0.909445 : CLUSTER: 5/5 matches (0.992484) - SPECTRUM: 5/5 matches (0.992604)
Matching ppm: 2.536, 2.559, 2.589, 2.665, 2.695
DBREF0001 (Aspartate) : Score=0.632789 : CLUSTER: 2/5 matches (0.984304) - SPECTRUM: 12/12 matches (0.825149)
Matching ppm: 2.665, 2.695
DBREF0017 (malic acid) : Score=0.587433 : CLUSTER: 2/5 matches (0.878619) - SPECTRUM: 8/12 matches (0.969622)
Matching ppm: 2.665, 2.695

NMR spectra viewer

- Examples online

  http://www.cbib.u-bordeaux2.fr/SPECNMR/examples



NMR spectra viewer

- Examples online http://www.cbib.u-bordeaux2.fr/SPECNMR/T06002