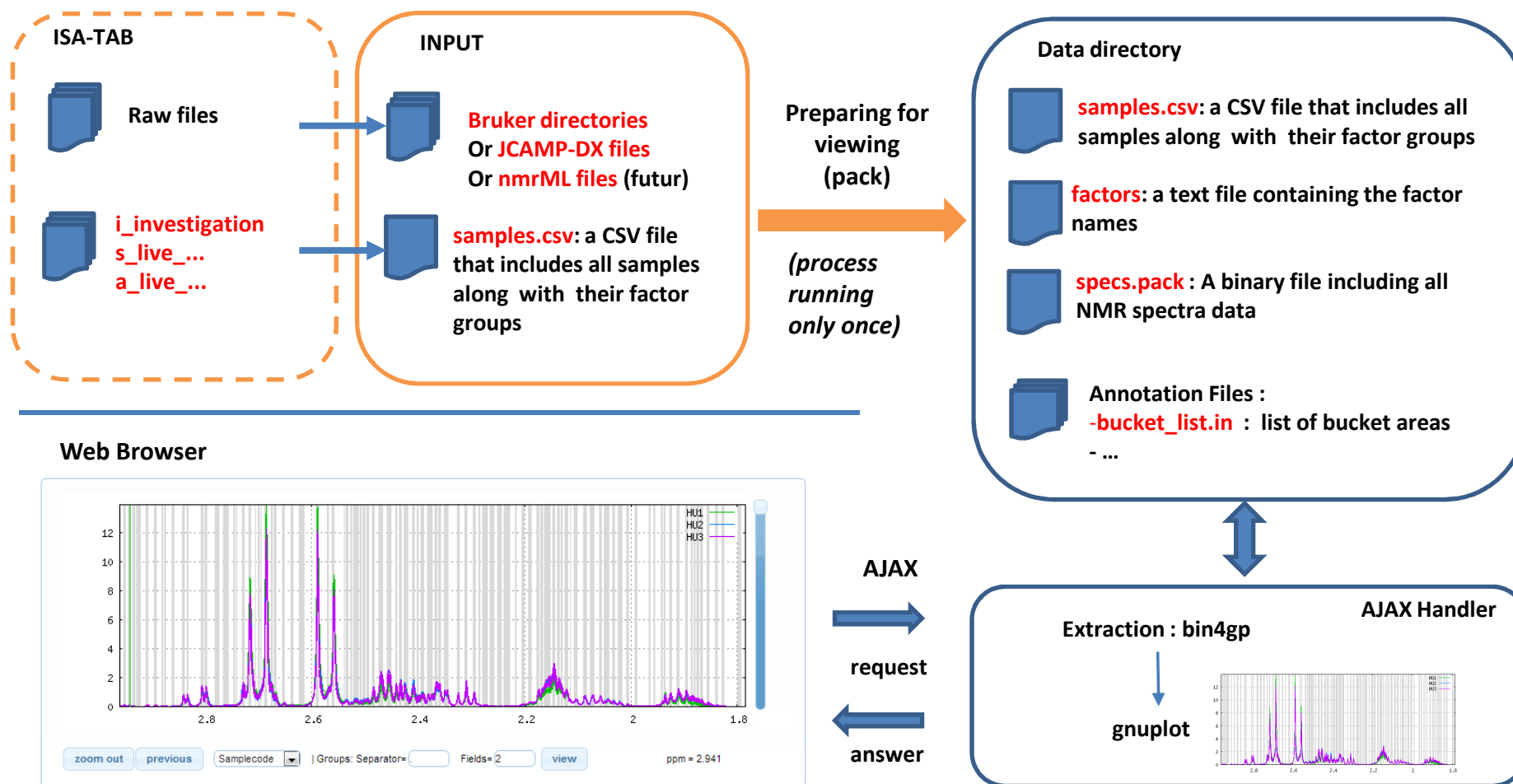


NMRViewer 1.0 - (C) INRA UMR 1332

Daniel Jacob

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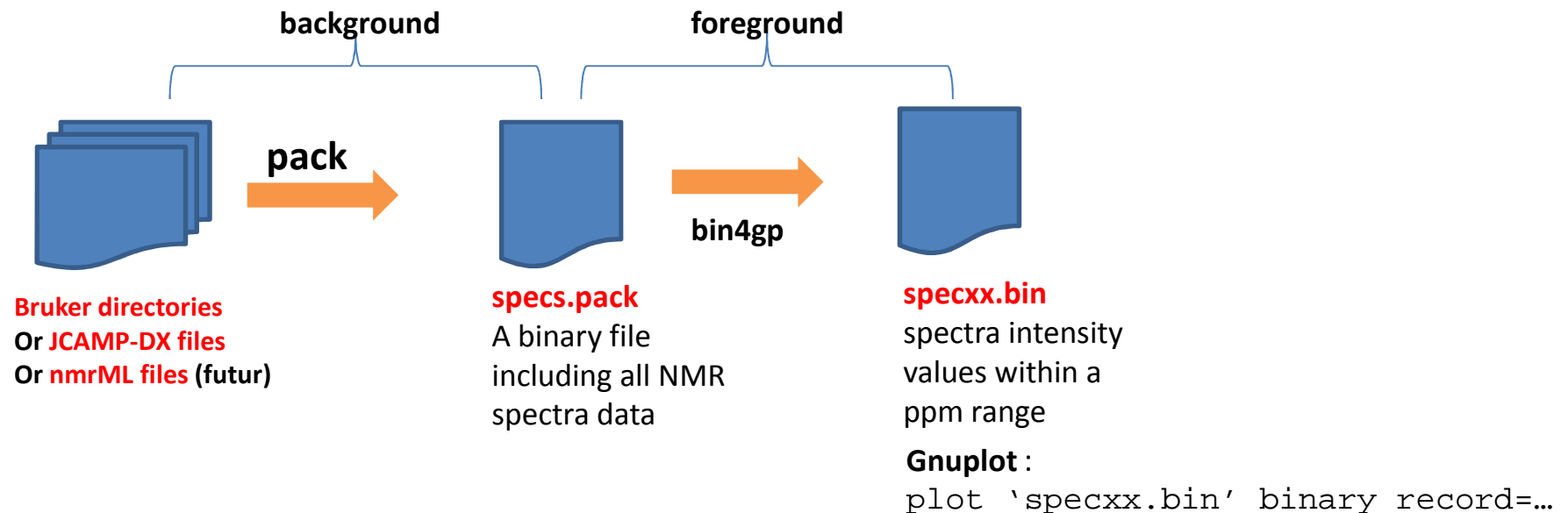
NMR spectra viewer : An overview of how it works



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.



➔ Trade off between consistency and efficiency

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
```

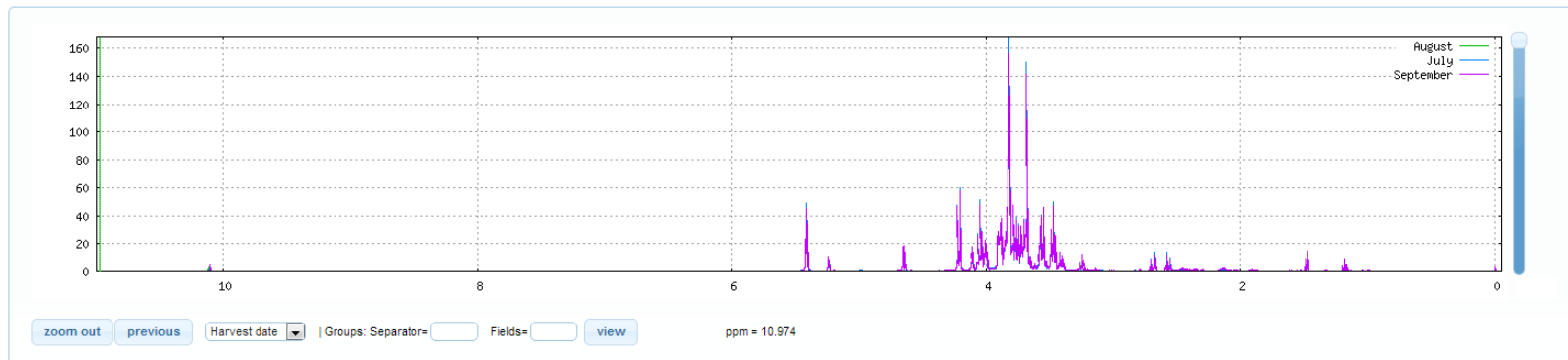
- Create the "pack" file

```
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>
```

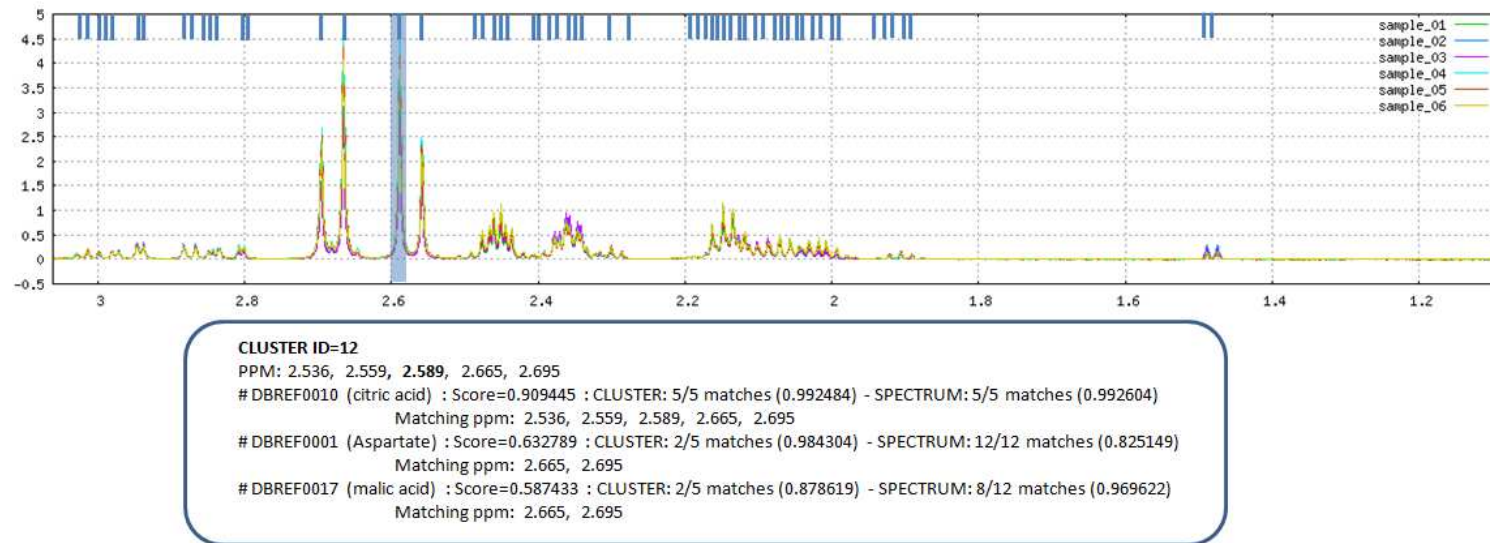


NMR spectra viewer : TODO

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%2Fs00216-013-6852-y](https://doi.org/10.1007%2Fs00216-013-6852-y))



NMR spectra viewer

- Examples online

<http://www.cbib.u-bordeaux2.fr/SPECNMR/test>

