

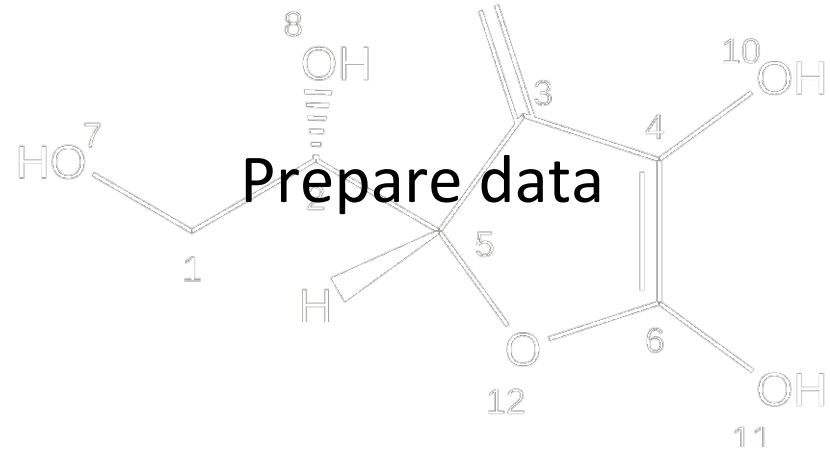


4 Wm

Workflow4metabolomics

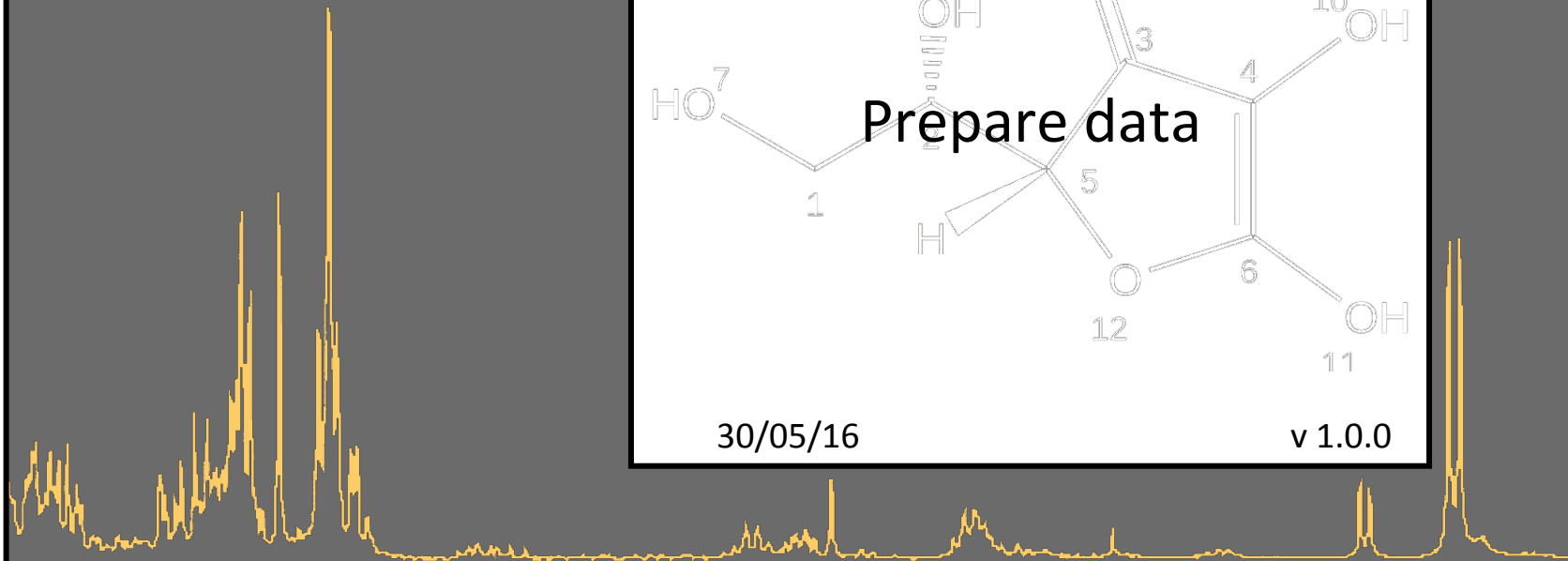


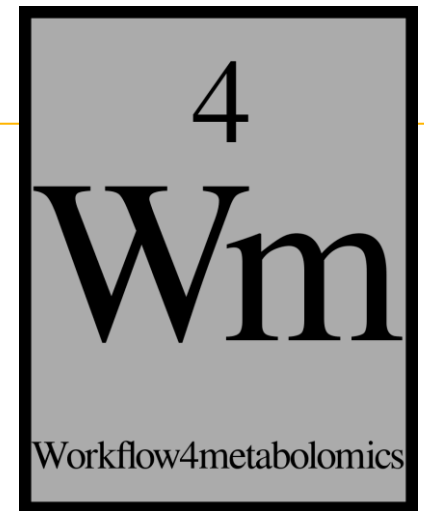
HOW TO



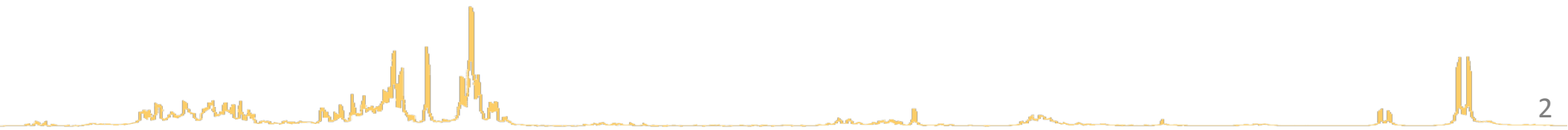
30/05/16

v 1.0.0





DATA FORMAT



Data format

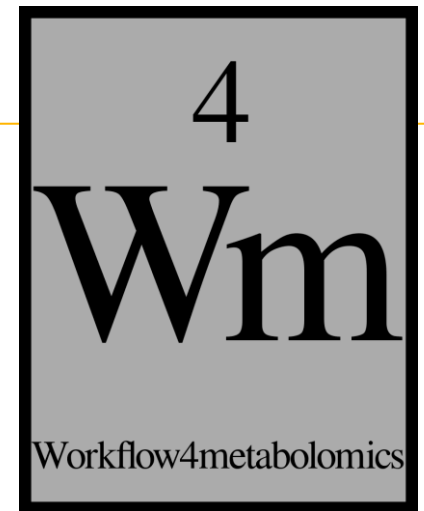
The XCMS package reads full-scan LC/MS data from AIA/ANDI format NetCDF, mzXML, and mzData files.

All data to be analyzed by XCMS must first be converted to one of those file formats.

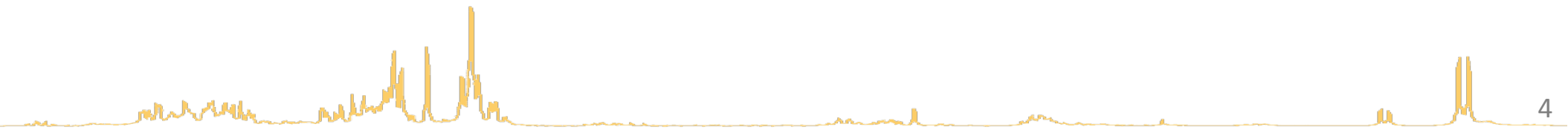
- Software packages for many instruments are able to export to NetCDF. For information about how to export to NetCDF, please consult the documentation that came with your instrument's software. Note that, the online help of most packages frequently use the terms "CDF" or "AIA" when referring to NetCDF format.
- mzXML exporters for a number of instruments are also available:
http://sashimi.sourceforge.net/software_glossolalia.html

source:

<http://bioconductor.org/packages/release/bioc/vignettes/xcms/inst/doc/xcmsPreprocess.pdf>



DATA ORGANIZATION



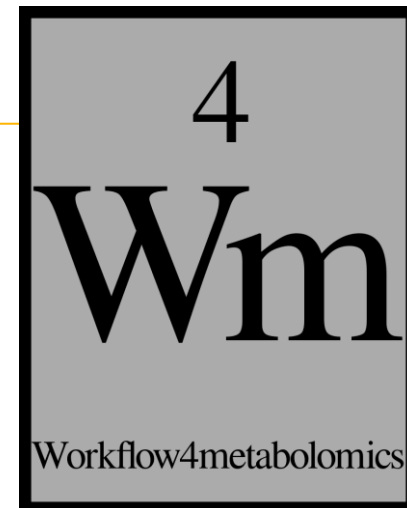
Data organization

If it's your case, your data must be segregated per condition in different folders

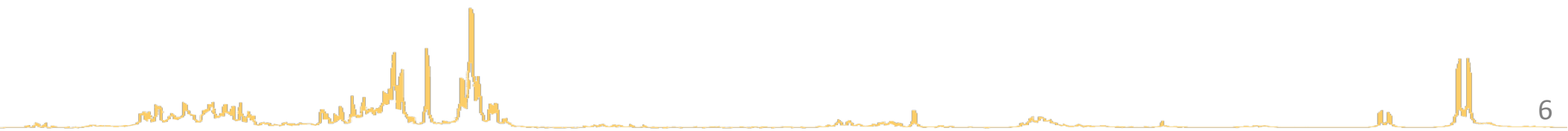
Example: sacuri/

- bio/
 - HU_neg_017.mzXML
 - HU_neg_028.mzXML
 - HU_neg_034.mzXML
- blank/
 - Blanc04.mzXML
 - Blanc06.mzXML
 - Blanc09.mzXML

Advise: avoid special characters in your filenames and path.



ZIP THE DATA



Zip the data

In order to keep the directory structure intact, we chose the usual Zip format.

Unfortunately, the zip utility available by default with Microsoft **Windows** produces some corrupted file if the size of your data is more than **4Go**.

So if you get this **error** message after the upload of your data

```
zipfile.BadZipfile: zipfiles that span multiple disks are not supported
```

Our advice is to use the file archiver **7ZIP** (<http://www.7-zip.org>)

