

Mass spectrometry and Free Software in Debian

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Mass spectrometry:

- ▶ Uses in the biochemical sciences;
- ▶ Cultural differences with other disciplines;
- ▶ Why free software is ever more considered essential;
- ▶ Software available in Debian and other packaging work.

A mass spectrometer

Source, analyser and detector (ion counter)

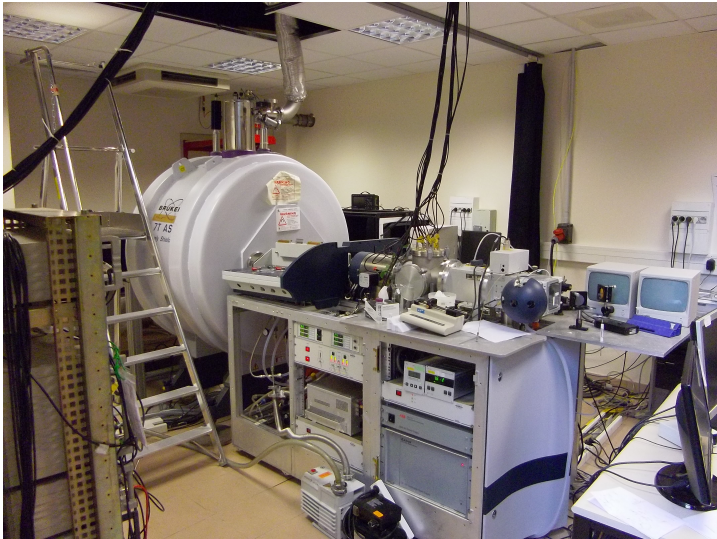
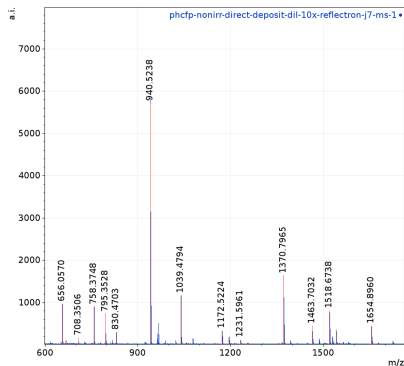


Photo: Vincent Steinmetz (U-Psud, Orsay)

A mass spectrum

Detected ion masses *versus* the count of the ions



- ▶ Proteins, DNA | RNA, Sugars → function and regulation (disease understanding);
- ▶ The applied sciences (big pharma) → drug development needs checking at the cell level the effect of a given drug. Mass spec shows the changes occurring upon treatment.

Why is Free Software so important here?

In the context of mass spectrometry for biology?

Hardware manufacturers are fiercely struggling to gain exclusive control both on the mass data and on the users themselves...

(“vendor lock-in”)

- ▶ Software is used as a sales pitch (particularly, LIMS[†]);
- ▶ Proprietary formats lock terabytes of (sensitive) data;
- ▶ Inter-project interoperability is hindered by the file format wars;
- ▶ MS facility users cannot themselves analyze their data;
- ▶ ⇒ Always ask for an “Export to mzML”[‡] feature.

[†] Laboratory Information Management System.

[‡] Or, at least, to a simple (x,y) format.

Cultural differences with other disciplines

Popularization of biopolymer mass spectrometry is recent

Genomics/Bioinformatics Old-style biochemistry

- ▶ Mid 1970's: sequencing of proteins/nucleic acids
⇒ simple-text raw data
⇒ rather easy data processing;
- ▶ PDP-11, VAX/VMS, DEC-ALPHA, UNIX...
- ▶ Easy text-based formatted-data display.

Mass spectrometry New-age hyper-technicity

- ▶ Mid 2000's: popularity of mass spectrometry
⇒ (x,y) text raw data
⇒ more complex data processing;
- ▶ MS-Windows NT4, Millennium, 2000...
- ▶ Complex graphics-based formatted-data display.

These chrono-technological differences impacted the unconscious computer-based behaviour of scientists

Since a few years, I see a behavioural shift...
that might foreshadow a mindset transition...

Pride in stating:

- ▶ *“Developed under GNU/Linux with FREE SOFTWARE;”*
- ▶ *“We can use tens of computers; spending nothing in licenses;”*

But not yet something like:

- ▶ *“We packaged our soft and set up a public repos;”*
 - ▶ *“How about having a powerful environment for both mass spec-centric software development and data analysis?”*
- ⇒ This is the proper time window to push *freedom* forward

Debian as a full-featured mass spectrometry setup?

Three kinds of users

- ▶ The massist — acquires the data and handles them:
 - ▶ Databases;
 - ▶ Nicely crafted site-specific workflows;
 - ▶ Some reporting.
- ▶ The user — a biologist (or else) mainly willing to click:
 - ▶ Nicely crafted application-specific number crunching;
 - ▶ Reporting tools;
- ▶ The developer: the guy willing to help the former.
 - ▶ Interfacing with databases (*i.e.* web interfaces);
 - ▶ Number-crunching coding C/C++/Python/Java;
 - ▶ Build systems (CMake, GNU autotools, bjam. . .);
 - ▶ Documentation-generation tools (sgml, LaTeX, TexInfo);

Debian source (binary) packages for mass spectrometry

- ▶ Before 2002: nothing;
- ▶ Since my switching to Debian:
 - ▶ `polyxmass` (2) and `massxpert` (3)
 - ▶ `lutefisk` (1)
 - ▶ `mmass` (2)
- ▶ Since a recent push to package new stuff:
 - ▶ libraries as tools to craft specific workflows:
 - ▶ `openms` (5)
 - ▶ `libpwiz` (3)
 - ▶ `tandem-mass` (1)
 - ▶ libraries/executables to handle data (format conversion, quantitation...):
 - ▶ `python-mzml` (2)
 - ▶ `r-cran-readbrukerflexdata` (1)
 - ▶ `r-cran-malDIquant` (1)

One example of a large software project

OpenMS (<http://open-ms.sourceforge.net/>)

- ▶ C++; LGPL 2.1; CMake-based;
- ▶ 2 libraries (fundamental and GUI);
- ▶ 114 binaries;
- ▶ Large documentation;
- ▶ **contrib** directory stuff with external libraries;
- ▶ “Hackish” DESTDIR-based design decisions to be revisited;
- ▶ Useful interactions with various project members;
- ▶ Build-Depends: debhelper ($\geq 7.0.50$), dpkg-dev ($\geq 1.16.1$), quilt ($\geq 0.60-2$), cmake ($\geq 2.6.3$), libxerces-c-dev ($\geq 3.1.1$), libgsl0-dev ($\geq 1.15+dfsg$), libboost1.49-dev, libboost-iostreams1.49-dev, libboost-date-time1.49-dev, libboost-math1.49-dev, seqan-dev ($\geq 1.3.1$), libsvm-dev (≥ 3.12), libglpk-dev (≥ 4.45), zlib1g-dev ($\geq 1.2.7$), libbz2-dev ($\geq 1.0.6$), cppcheck (≥ 1.54), libqt4-dev ($\geq 4.8.2$), libqt4-opengl-dev ($\geq 4.8.2$), libqtwebkit-dev ($\geq 2.2.1$), coinor-libcoinutils-dev ($\geq 2.6.4$), imagemagick, doxygen ($\geq 1.8.1.2$), texlive-extra-utils, texlive-latex-extra, latex-xcolor, texlive-font-utils, ghostscript, texlive-fonts-recommended

Using Debian for such a project — PROS...

- ▶ Huge amount of pre-packaged software (libraries, particularly);
- ▶ Basis of many derivatives;
- ▶ Debian Pure Blends infrastructure (*Debichem*);
- ▶ Wonderful and welcoming infrastructure for collaborative packaging (alioth.debian.org);
- ▶ Robustness of the *stable* (even *testing*) distributions;

Using Debian for such a project — CONS...

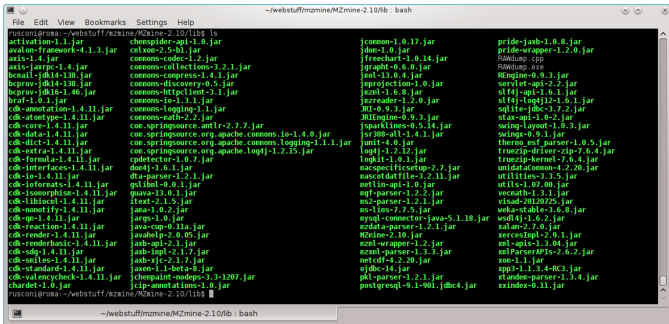
- ▶ Packaging is highly involved and may hinder the involvement of colleagues who do not want to invest too much time. Mentoring plays a *huge* role here;
- ▶ Intimidating distribution for the average biochemist (specifically at install time). This should become ever less true with the installer progress since some time;

Challenges...

Rocky packaging ahead...

Java-based sophisticated mass spectrum viewer at

<http://mzmine.sourceforge.net>



```
~/webstuff/mzmine/MZmine-2.10.10b : bash
File Edit View Bookmarks Settings Help
rusccon@ora1 ~$ ls
activation-1.1.jar      commons-collections-3.2.1.jar  commons-logging-1.1.jar
avalon-framework-4.1.3.jar  commons-codesc-1.2.jar        commons-math-2.2.jar
axis-1.4.jar            commons-httpclient-3.1.jar     com.springsource.antlr-2.7.7.jar
axis-jaxrpc-1.4.jar      commons-io-1.3.1.jar          com.springsource.org.apache.commons.io-1.4.0.jar
bcmail-jdk14-138.jar     commons-net-3.1.jar           com.springsource.org.apache.commons.logging-1.1.1.jar
bcprov-jdk14-138.jar     commons-pool-1.5.6.jar        com.springsource.org.apache.log4j-1.2.15.jar
bcprov-jdk16-1.46.jar    commons-rmi-2.0.jar           cpdetector-1.0.7.jar
brat-1.0.1.jar           commons-logging-1.1.jar       dnet1-1.0.1.jar
cdk-annotation-1.4.11.jar  commons-math-2.2.jar          dta-parser-1.2.1.jar
cdk-atontype-1.4.11.jar   com.springsource.org.apache.commons.io-1.4.0.jar  gslib-0.0.1.jar
cdk-core-1.4.11.jar      com.springsource.org.apache.commons.logging-1.1.1.jar  guava-13.0.1.jar
cdk-datas-1.4.11.jar     commons-net-3.1.jar           hext-2.1.5.jar
cdk-dict-1.4.11.jar      commons-pool-1.5.6.jar        jama-1.0.2.jar
cdk-extra-1.4.11.jar     commons-rmi-2.0.jar           jargs-1.0.jar
cdk-formula-1.4.11.jar   commons-logging-1.1.jar       java-cup-0.11a.jar
cdk-interfaces-1.4.11.jar  commons-math-2.2.jar          javahelp-2.0.05.jar
cdk-io-1.4.11.jar        com.springsource.org.apache.commons.io-1.4.0.jar  jaxb-api-2.1.jar
cdk-ioformats-1.4.11.jar  com.springsource.org.apache.log4j-1.2.15.jar  jaxb-impl-2.1.7.jar
cdk-isomorphisms-1.4.11.jar  cpdetector-1.0.7.jar          jaxb-rt-2.1.7.jar
cdk-libhsca-1.4.11.jar    dnet1-1.0.1.jar              jaxml-1.3-beta-8.jar
cdk-notify-1.4.11.jar     dta-parser-1.2.1.jar          jchempaint-nodesp-3.3-1207.jar
cdk-qn-1.4.11.jar        gslib-0.0.1.jar              jclip-annotations-1.0.jar
cdk-reaction-1.4.11.jar  guava-13.0.1.jar             jcommon-1.0.17.jar
cdk-render-1.4.11.jar    hext-2.1.5.jar               jdon-1.0.jar
cdk-renderbasic-1.4.11.jar  jama-1.0.2.jar               jfreechart-1.0.14.jar
cdk-sdg-1.4.11.jar       jargs-1.0.jar                jgraph-0.6.0.jar
cdk-smiles-1.4.11.jar    java-cup-0.11a.jar           jmol-13.0.4.jar
cdk-standards-1.4.11.jar  javahelp-2.0.05.jar          jsprojection-1.0.jar
cdk-valencycheck-1.4.11.jar  jaxb-api-2.1.jar            jszip-1.6.8.jar
chardet-1.0.jar          jaxb-impl-2.1.7.jar         jzrender-1.2.0.jar
ruscon@ora1 ~$ ls
activation-1.1.jar      commons-collections-3.2.1.jar  commons-logging-1.1.jar
avalon-framework-4.1.3.jar  commons-codesc-1.2.jar        commons-math-2.2.jar
axis-1.4.jar            commons-httpclient-3.1.jar     com.springsource.antlr-2.7.7.jar
axis-jaxrpc-1.4.jar      commons-io-1.3.1.jar          com.springsource.org.apache.commons.io-1.4.0.jar
bcmail-jdk14-138.jar     commons-net-3.1.jar           com.springsource.org.apache.commons.logging-1.1.1.jar
bcprov-jdk14-138.jar     commons-pool-1.5.6.jar        com.springsource.org.apache.log4j-1.2.15.jar
bcprov-jdk16-1.46.jar    commons-rmi-2.0.jar           cpdetector-1.0.7.jar
brat-1.0.1.jar           commons-logging-1.1.jar       dnet1-1.0.1.jar
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cdk-core-1.4.11.jar      com.springsource.org.apache.commons.logging-1.1.1.jar  guava-13.0.1.jar
cdk-datas-1.4.11.jar     commons-net-3.1.jar           hext-2.1.5.jar
cdk-dict-1.4.11.jar      commons-pool-1.5.6.jar        jama-1.0.2.jar
cdk-extra-1.4.11.jar     commons-rmi-2.0.jar           jargs-1.0.jar
cdk-formula-1.4.11.jar   commons-logging-1.1.jar       java-cup-0.11a.jar
cdk-interfaces-1.4.11.jar  commons-math-2.2.jar          javahelp-2.0.05.jar
cdk-io-1.4.11.jar        com.springsource.org.apache.commons.io-1.4.0.jar  jaxb-api-2.1.jar
cdk-ioformats-1.4.11.jar  com.springsource.org.apache.log4j-1.2.15.jar  jaxb-impl-2.1.7.jar
cdk-isomorphisms-1.4.11.jar  cpdetector-1.0.7.jar          jaxb-rt-2.1.7.jar
cdk-libhsca-1.4.11.jar    dnet1-1.0.1.jar              jaxml-1.3-beta-8.jar
cdk-notify-1.4.11.jar     dta-parser-1.2.1.jar          jchempaint-nodesp-3.3-1207.jar
cdk-qn-1.4.11.jar        gslib-0.0.1.jar              jclip-annotations-1.0.jar
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cdk-renderbasic-1.4.11.jar  jama-1.0.2.jar               jfreechart-1.0.14.jar
cdk-sdg-1.4.11.jar       jargs-1.0.jar                jgraph-0.6.0.jar
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cdk-valencycheck-1.4.11.jar  jaxb-api-2.1.jar            jszip-1.6.8.jar
chardet-1.0.jar          jaxb-impl-2.1.7.jar         jzrender-1.2.0.jar
ruscon@ora1 ~$
```

- ▶ Non-free but highly useful software;
- ▶ Databases of natural data (undistributable);