A Parser for `nmrML`

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Contents

1 Introduction

The nmRIO package aims at providing a common interface to several NMR data formats.

Cool R packages for NMR processing are e.g. Lewis et al. (2009) and Hao et al. (2012)

2 Example

A short example sequence to read data from a mass spectrometer. First open the file.

```
> library(nmRIO)
> nmrMLfile <- system.file("examples/HMDB00005.nmrML", package = "nmRIO")
> fid <- readNMRMLFID(nmrMLfile)
>
```

```
> plot(Re(fid), type="l")
```

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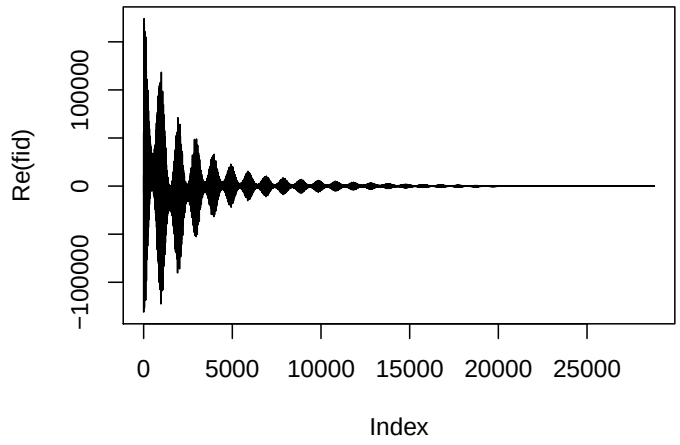
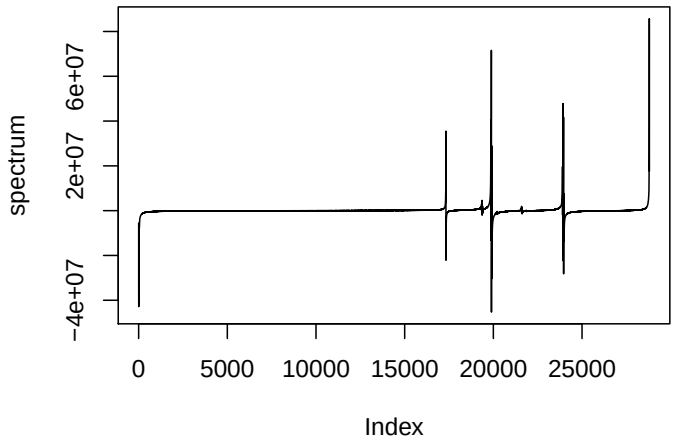


Luis: I also need to access the following parameters: spectral width (ideally in ppm but can work out the one in Hz) transmitter frequency. Later, for bruker files I also need the following data group delay, dsp firmware version

```
>   tree <- xmlTreeParse(nmrMLfile)
>   root <- xmlRoot(tree)
>   ## Get required parameters from nmrML
>   irradiationFrequency <- as.double(xmlAttrs(xmlElementsByTagName(root, "irradiationFreq
>   sweepWidth <- as.double(xmlAttrs(xmlElementsByTagName(root, "sweepWidth", recursive =
>   numberOfDataPoints <- as.integer(xmlAttrs(xmlElementsByTagName(root, "DirectDimensionP
>   irradiationFrequency

[1] 599.4094

>   sweepWidth

[1] 7200.072

>   numberOfDataPoints

[1] 57804

>   spectrum <- Re(fft(fid, inverse=TRUE))
```

The rudimentary processing results in:

```
> plot(spectrum, type="l")
```




```
> ## Mockup to write the spectrum back into the nmrML
> ## as "processed data"
>
> #b64string <- nmRIO:::binaryArrayEncode(spectrum, byteFormat="complex64", compression="g
>
```

3 Future plans

A lot.

4 Session information

- R version 3.1.1 (2014-07-10), `x86_64-pc-linux-gnu`
- Locale: `LC_CTYPE=en_US.UTF-8`, `LC_NUMERIC=C`, `LC_TIME=de_DE.UTF-8`, `LC_COLLATE=en_US.UTF-8`, `LC_MONETARY=de_DE.UTF-8`, `LC_MESSAGES=en_US.UTF-8`, `LC_PAPER=de_DE.UTF-8`, `LC_NAME=C`, `LC_ADDRESS=C`, `LC_TELEPHONE=C`, `LC_MEASUREMENT=de_DE.UTF-8`, `LC_IDENTIFICATION=C`
- Base packages: base, datasets, graphics, grDevices, methods, stats, utils
- Other packages: caTools 1.17, nmRIO 0.3, XML 3.98-1.1
- Loaded via a namespace (and not attached): bitops 1.0-6, tools 3.1.1

References

Jie Hao, William Astle, Maria De Iorio, and Timothy M D Ebbels. BATMAN–an R package for the automated quantification of metabolites from nuclear

magnetic resonance spectra using a Bayesian model. *Bioinformatics*, 28(15): 2088–2090, Aug 2012. doi: 10.1093/bioinformatics/bts308. URL `http://dx.doi.org/10.1093/bioinformatics/bts308`.

Ian A Lewis, Seth C Schommer, and John L Markley. rNMR: open source software for identifying and quantifying metabolites in NMR spectra. *Magn Reson Chem*, 47 Suppl 1:S123–S126, Dec 2009. doi: 10.1002/mrc.2526. URL `http://dx.doi.org/10.1002/mrc.2526`.