



**an HTML interface for displaying
the contents of NMReDATA files,
molecular structure, NMR data and
spectra**

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The aims: a viewer

Browse contents of NMReDATA files
(zipped package)

Work locally as well as over the web
(non disclosure may be needed)

Display contents of all NMReDATA tags
(inside the SDF file)

Display molecular structure
(both 2D and 3D, interactive)

Display NMR assignments and couplings on the
molecular structure

Display NMR spectra

The aims (II): an editor

Edit NMReDATA records

Generate a 3D structure for the given 2D

Optimised structure

Add implicit hydrogens

Correct stereochemistry

Add tags (both NMReDATA records and extra records, metadata...)

Add files to the package

Save modified package to a new file on disk

The tool

In a webpage: HTML5, JavaScript (no Java); local or web server

The screenshot displays the web-based NMReDATA editor interface. It features several main sections:

- File contents:** A file tree on the left showing the package structure, including folders like 'AN-menthol' and 'jcamp_nmr_spectra'.
- NMReDATA tags:** A central panel showing a list of tags such as VERSION, LEVEL, SOLVENT, and ASSIGNMENT, with their corresponding values.
- Molecular structure display:** A 3D ball-and-stick model of a molecule, with chemical shifts and coupling constants overlaid on the atoms.
- Spectra:** A plot of the 1H NMR spectrum, showing intensity versus chemical shift (PPM).

Additional features include a 'Save edited file' section, a 'Log of changes' section, and various control buttons for assignments, couplings, and file operations.

Files in package

Content of files

Structure display (JSmol)
Engine for data and file operations

Display of spectra (JSpecView) in JCAMP format

Features (I)

Display contents of several types

Structure

bond up / down

Chemical shifts, assignments and couplings are annotated over the molecular structure.

NMREDATA_ASSIGNMENT

restrict display: H, C, X, interchangeable

interchangeable and equivalent (colour coded)

NMREDATA_J

explicit / implicit

may restrict display: HH, HX, XX, >3Hz

from J tag or from 1D spectra

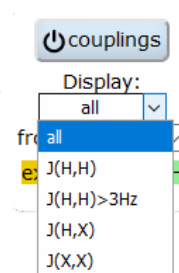
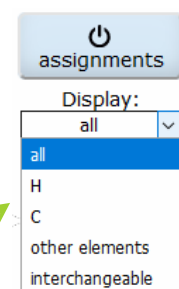
Edition of tag contents

reads both versions <1 & >1

automatic processing of line terminator

allows for comments

Addition of new tags



Features (II)

Obtain a 3D structure from the 2D formula

Using JSmol:

Adds implicit H's

Keeps assignments and couplings (modified as needed)

Manually assisted to obtain correct stereo

Manual assignation of interchangeable and equivalent pairs

Using the ALATIS server

Retrieves key and InChI that may be added to the data set

Adds implicit H's

Breaks assignments ☹️

Stereo cannot be controlled ☹️

3D is added to the file as a 2nd model in the SDF

Features (III)

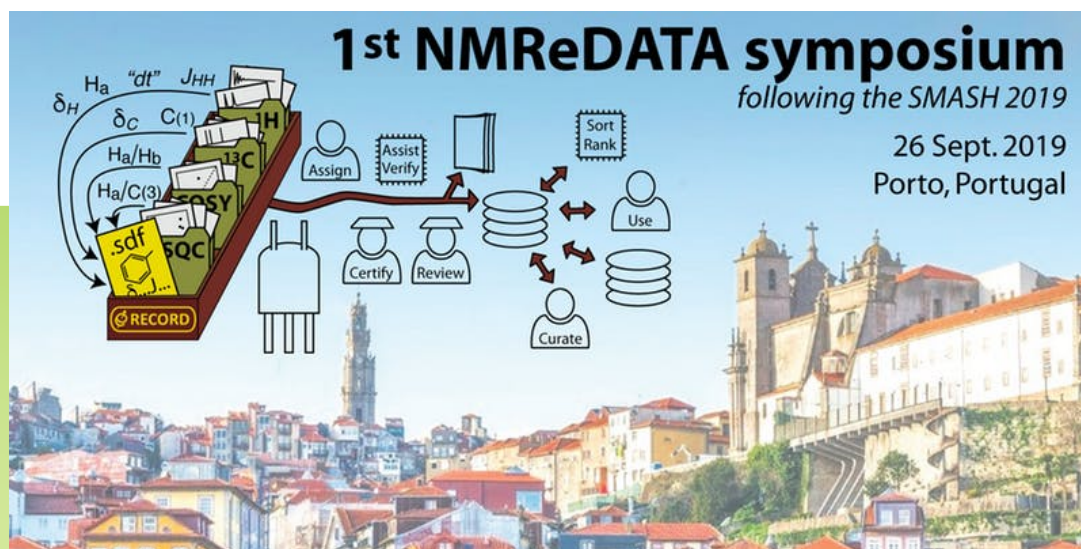
Modifying the package

Add files

Remove files

Save modified package to local disk

Changes (tags, 3D model, files) are logged and the log saved as part of the modified package



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http://www3.uah.es/nmr_e_data/

