NMR DATA J-reader

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

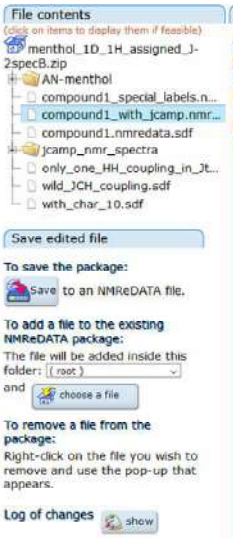
Add tags (both NMReDATA records and extra records, metadata...)

Add files to the package

Save modified package to a new file on disk

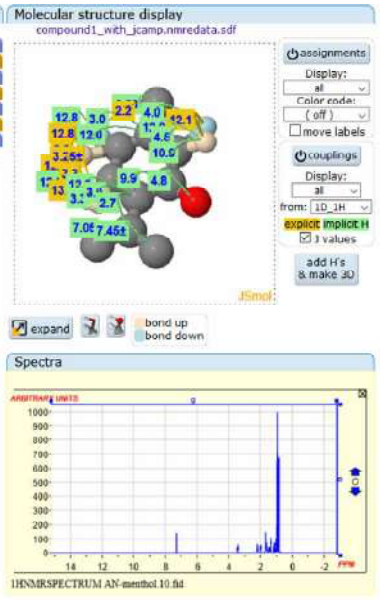
The tool

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



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)

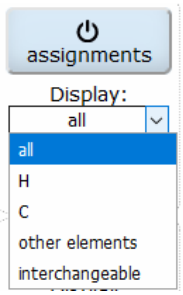
NMREDATA_J

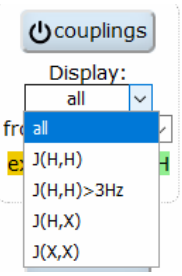
- explicit / implicit
- may restrict display: HH, HX, XX, >3Hz
- from J tag or from 1D spectra

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 ☹

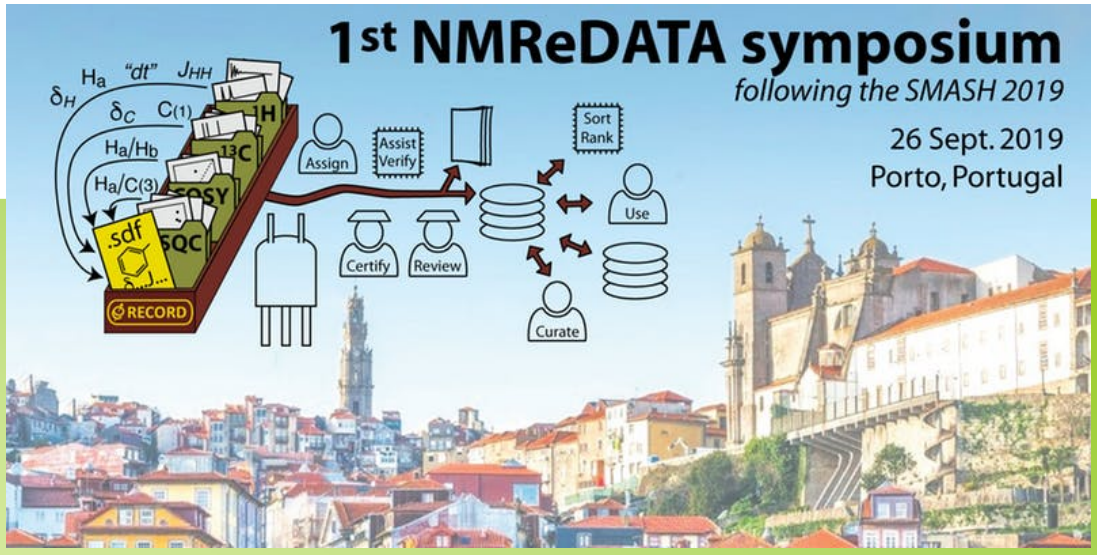
3D is added to the file as a 2nd model in the SDF

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/