NMReDATA software and nmrshiftdb2

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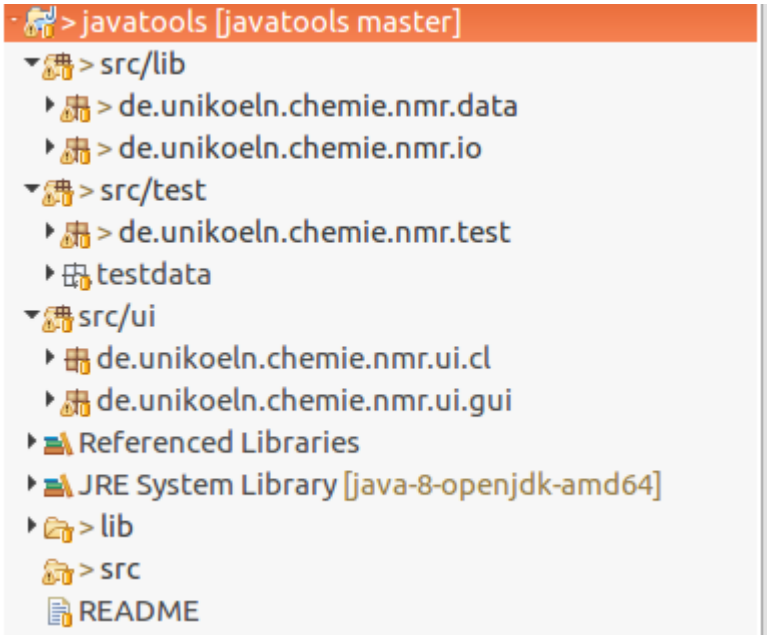
Overview

- The NMReDATA tools
- Standalone functions
- Use as library
- Example: LDS
- nmrshiftdb2

The Java tools library

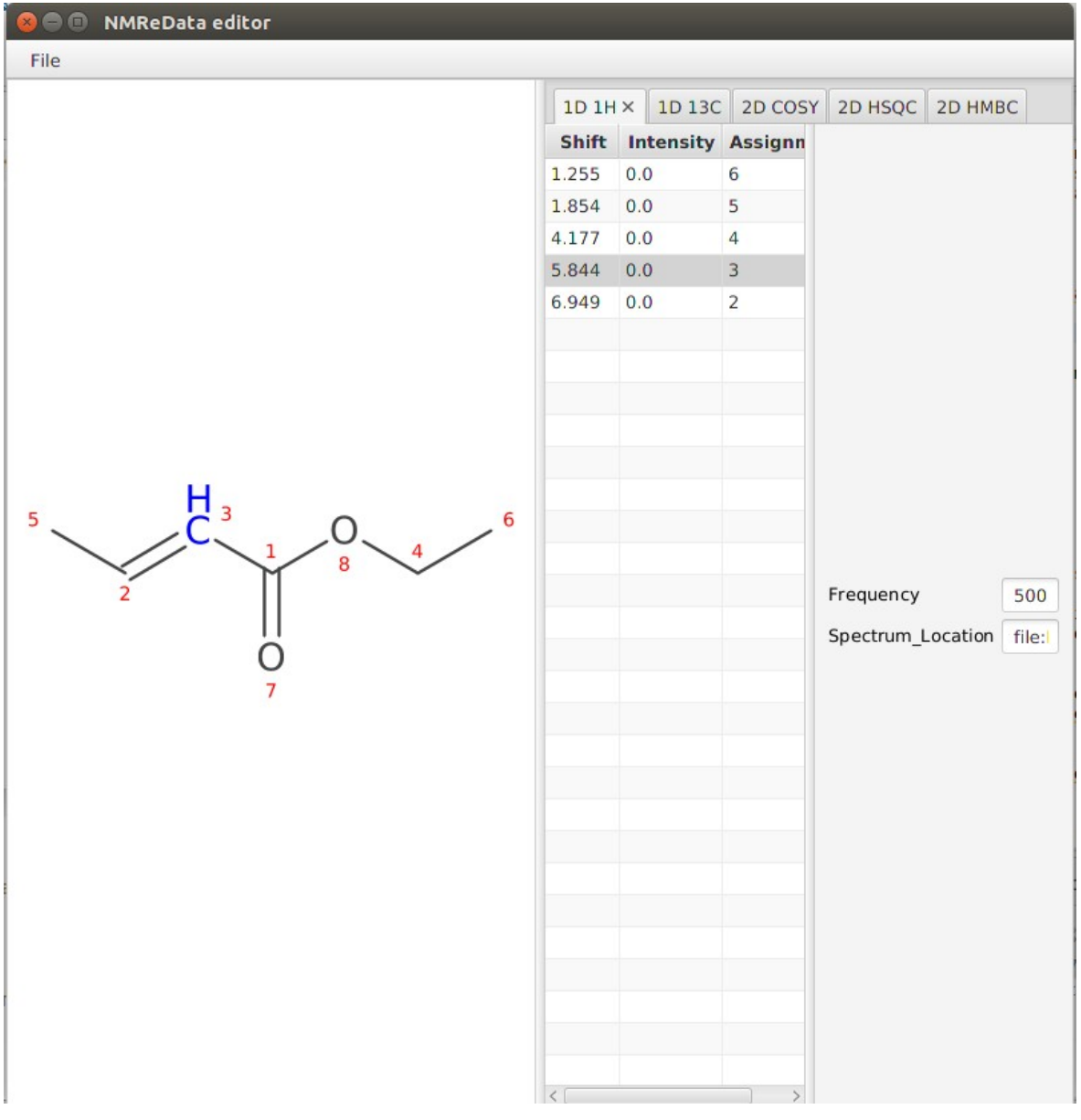
- NMReDATA java tools contain a java library for reading and writing NMReDATA files
- Internal object come from the jcamp-dx library
- Allows direct reading/writing as jcamp
- Programs can integrate the library and navigate the object tree
- Also serves as conformity check

https://github.com/NMReDATA Initiative/javatools



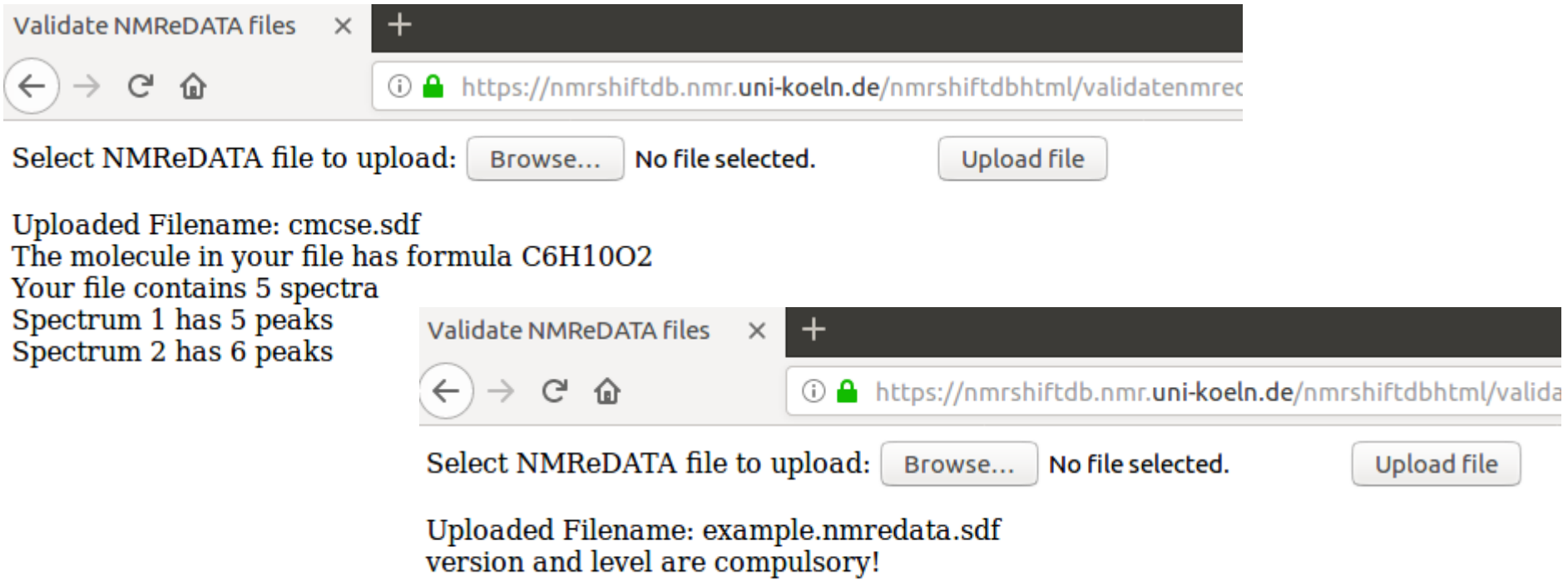
The Java tools library

- Offers command line and GUI interface
- GUI allows opening, viewing and saving as NMReDATA, LSD or jcamp, editing and more data formats will follow



The Java tools library

- Integration into web applications is possible
- Online check is at https://nmrshiftdb.nmr.uni-koeln.de/nmrshiftdbhtml/validatenmredata.jsp



The Java tools library

- Can be integrated in other products
- Example: LSD
- Has its own format, not very complicated
- 65 lines of code in Java tools make them write LSD files

```
C:\Users\Privat#\Desktop\LSDos-3.4.10>lsdnmredata.bat "HAP_benzo(a)pyrene_assign
ments_1.nmredata.sdf"
Converting NMReDATA file to LSD file...
…
1 solution found.
Result written to "HAP_benzo(a)pyrene_assignments_1.nmredata.sdf".sol.sdf

C:\Users\Privat#\Desktop\LSDos-3.4.10>lsdnmredata.bat cmcse.sdf
Converting NMReDATA file to LSD file...
…
1 solution found.
Result written to cmcse.sdf.sol.sdf
```

nmrshiftdb2

NMReDATA (by using the Java tools) has been integrated into nmrshiftdb2 for the following functions:

- Loading data into QuickCheck and assignment tool
- Submitting data
- Downloading data (original file as well as generated, NMR Record is possible as well)
- Downloading the database as NMReDATA

Nmrshiftdb2 - QuickCheck

Choose an MNova mol or sd file (MNova 11 or newer) or ChemDraw mol file with labels:
Browse... No file selected.
Choose a Topspin zip file including a CMC-SE result: Browse... No file selected.
Choose an NMReDATA file: Browse... cmcse.sdf
Clear form Transfer

Atom	δ [ppm]	Deviation from prediction
1	166.603	0.30
2	144.493	0.34
3	122.699	0.35
4	60.151	0.25
5	17.98	0.08
6	14.166	0.07

Home Search Results Quick Check Predict Assignment Submit Review Help

Quick Check
Note that this feature is currently experimental!

If you **login**, your Quick Check results will be available later!

Import from structures history

Choose an MNova mol or sd file (MNova 11 or newer) or ChemDraw mol file with labels:
Browse... No file selected.
Choose a Topspin zip file including a CMC-SE result: Browse... No file selected.
Choose an NMReDATA file: Browse... No file selected.

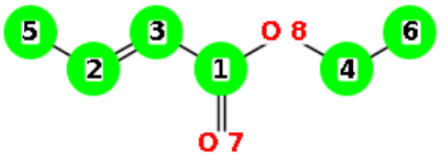
1D spectra | 2D spectra

Atom No.	^{13}C Shift		^{1}H Shift		
1	166.603	Keep unchanged			
	166.30, diff: 0.30				
2	144.493	Keep unchanged	H9	6.949	Keep unchange
	144.15, diff: 0.34			6.95, diff: 0.00	
3	122.699	Keep unchanged	H10	5.844	Keep unchang
	123.05, diff: 0.35			5.82, diff: 0.02	
4	60.151	Keep unchanged	H11	4.177	Keep unchang
	59.90, diff: 0.25			4.16, diff: 0.02	
5	17.98	Keep unchanged	H13	1.854	Keep unchang
	17.90, diff: 0.08			1.86, diff: 0.01	
6	14.166	Keep unchanged	H16	1.255	Keep unchang
	14.24, diff: 0.07			1.22, diff: 0.04	

If your structure has more atoms, transfer to get more fields!
*=symmetrical atom, if left empty it will be filled in automatically

Submit ^{13}C — Input list: Input format
Submit ^{1}H — Input list: Input format

Use .SHIFT REFERENCE in jcamp files (e. g. files from Topspin)



10: nmrshiftdb2 quality check: accept/reliability: excellent

Nmrshiftdb2 – Submitting data

Choose an MNova mol or sd file (MNova 11 or newer) or ChemDraw mol file with labels: Browse... No file selected.

Upload

Choose a Topspin zip file including a CMC-SE result: Browse... No file selected.

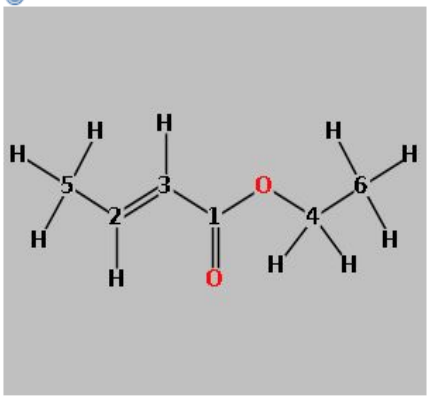
Upload

Choose an NMReDATA file: Browse... cm

Upload

Abort **Submit Data**

Choose your spectrum type!



Spectrum type: 13C

Atom No. ⇓	Shift	Mult. (coupling const.)
1	166.603	
2	144.493	
3	122.699	
4	60.151	
5	17.98	
6	14.166	

Chemical name(s):
Double Bond Specification:
CAS number:
Conditions:
Additional comments:
Additional spectrum information:
Spectrum keywords:
No JCAMP-DX file attached!
No PDF file attached!
No raw data file attached!
No image file attached!
No other files attached!

Export your submit (does not save or finish the submit):

Get this molecule as svg file Request

Get this spectrum as svg file Request

Get this spectrum and its molecule as simple html

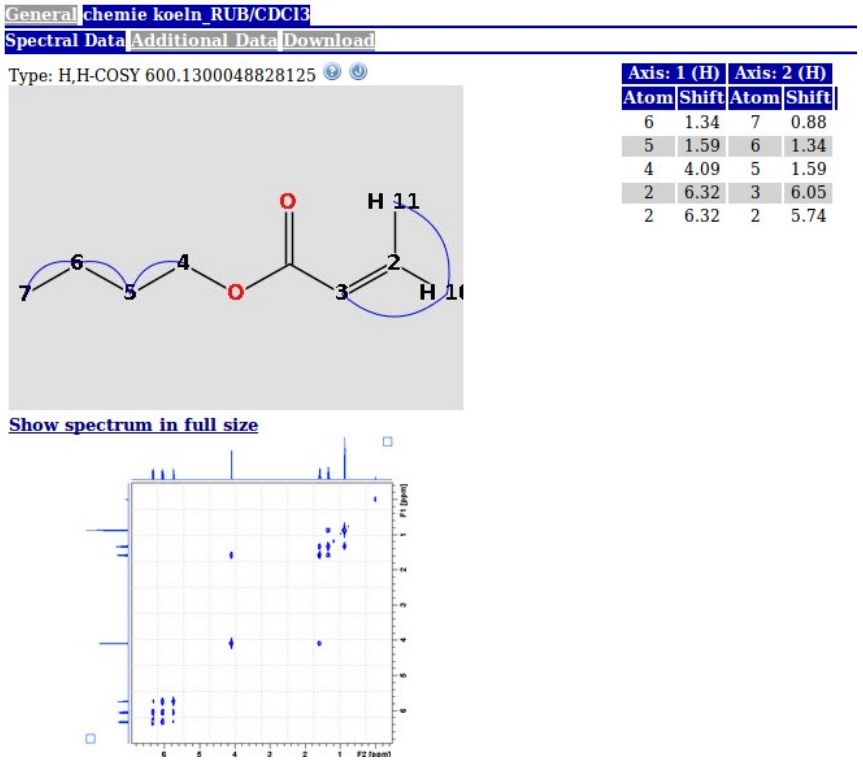
Enter molecule → Setting spectrum type → Add shifts → Do assignment → Add miscellaneous data → Add literature items → Attach files → Final submit

Your Mnova or Topspin file contains the spectrum types given below. Choose which one you want to submit now. You submit the other spectrum by uploading the file again, if you have not yet done both! Spectrum type:

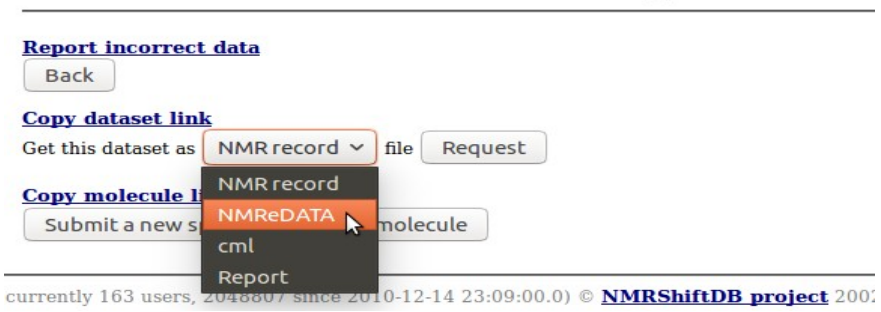
13C Submit spectrum type

Abort this submit

Nmrshiftdb2 – Downloading data



...



Nmrshiftdb2 – Downloading the database (available soon)

File	Date	Author	Commit
.project	2015-09-05	shk3	[r948] new predictor jars
nmrshiftdb2.sd	2019-04-25	shk3	[r1876] 2019-04-25
nmrshiftdb2.xml	2019-04-25	shk3	[r1876] 2019-04-25
nmrshiftdb2_3d.sd	2019-04-25	shk3	[r1876] 2019-04-25
nmrshiftdb2_3d.xml	2019-04-25	shk3	[r1876] 2019-04-25
nmrshiftdb2datalicense.txt	2015-09-01	shk3	[r942] 2015-09-01
nmrshiftdb2withsignals.sd	2019-04-25	shk3	[r1876] 2019-04-25
nmrshiftdb2withsignals_3d.sd	2019-04-25	shk3	[r1876] 2019-04-25
predictorc.jar	2019-07-30	shk3	[r1929] predictor jars with 3d hose codes
predictorh.jar	2019-07-30	shk3	[r1929] predictor jars with 3d hose codes

Conclusions

- The NMReData Java tools offer a possibility to view, check, and convert NMReDATA files
- They can be integrated easily into other programs
- By integrating them into nmrshiftdb2, NMReDATA can be imported and exported to nmrshiftdb2
- This enables easy integration of data sources