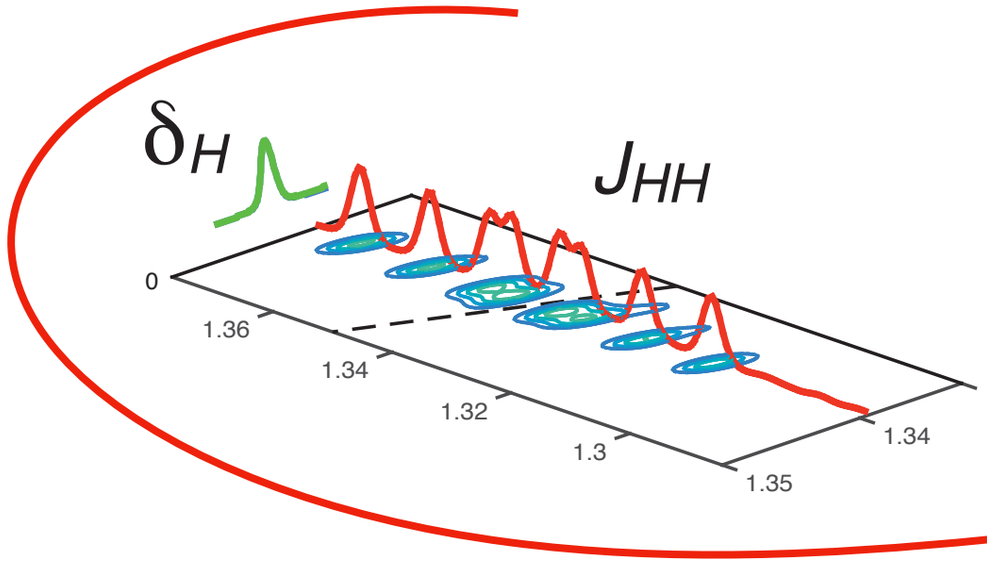
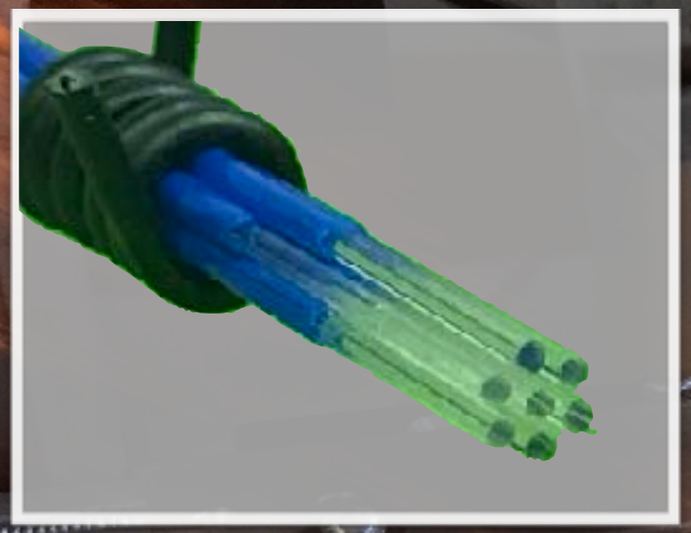
NMReDATA: a format and a good practice to exchange NMR parameters associated to chemical structures

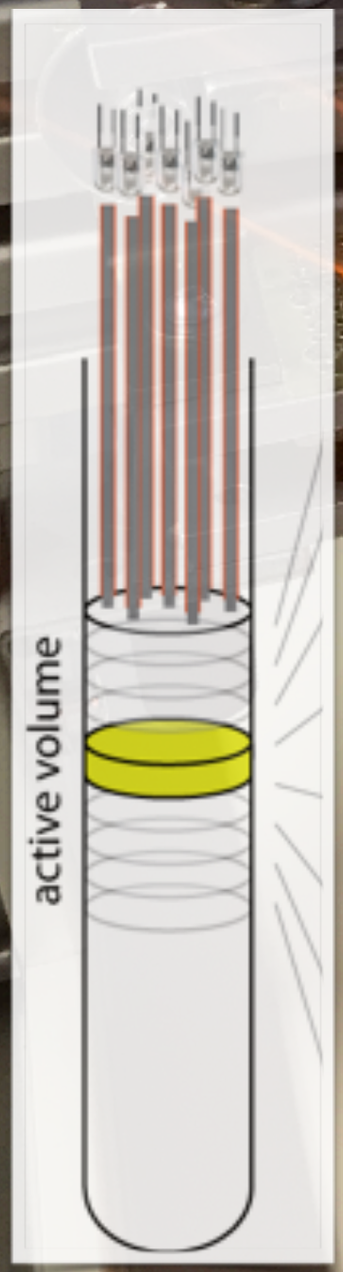


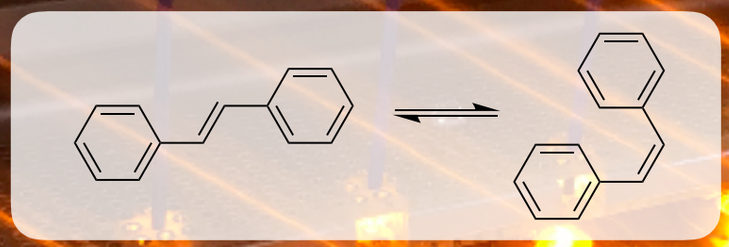
Damien Jeannerat

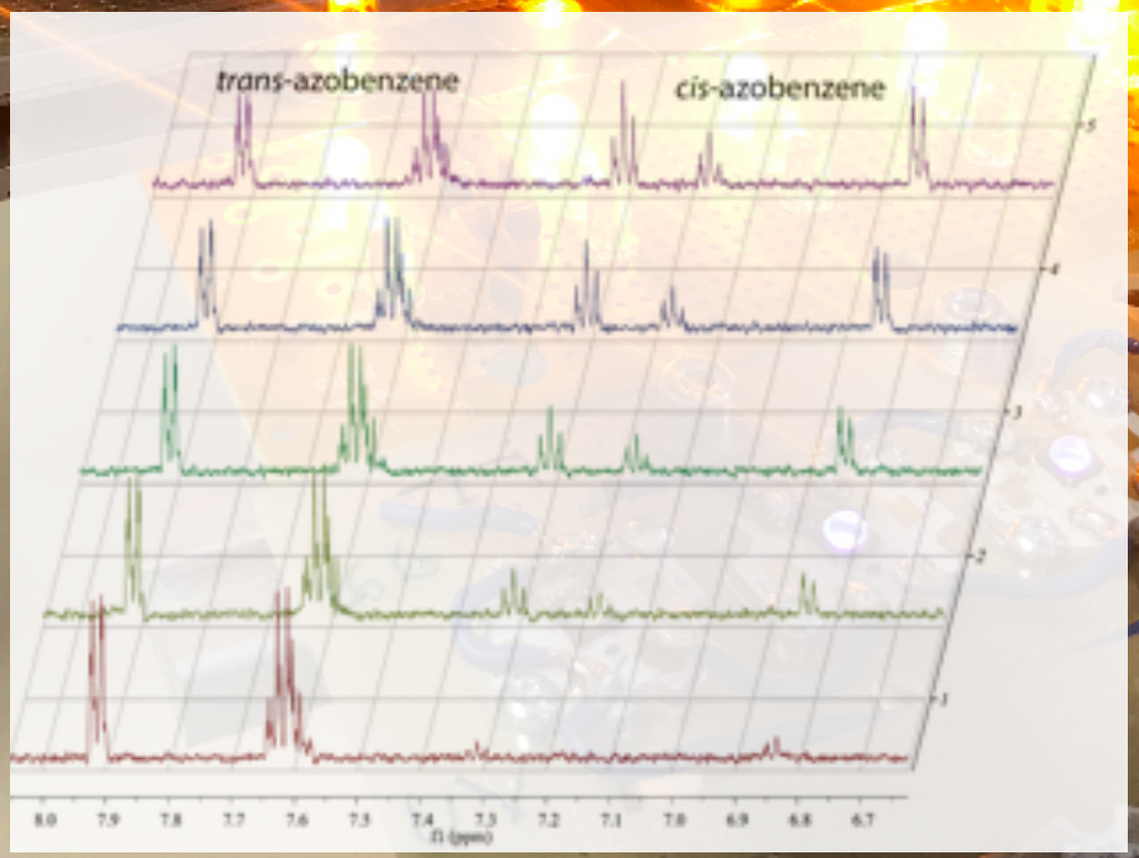
Departement of Organic Chemistry,

University of Geneva, Switzerland



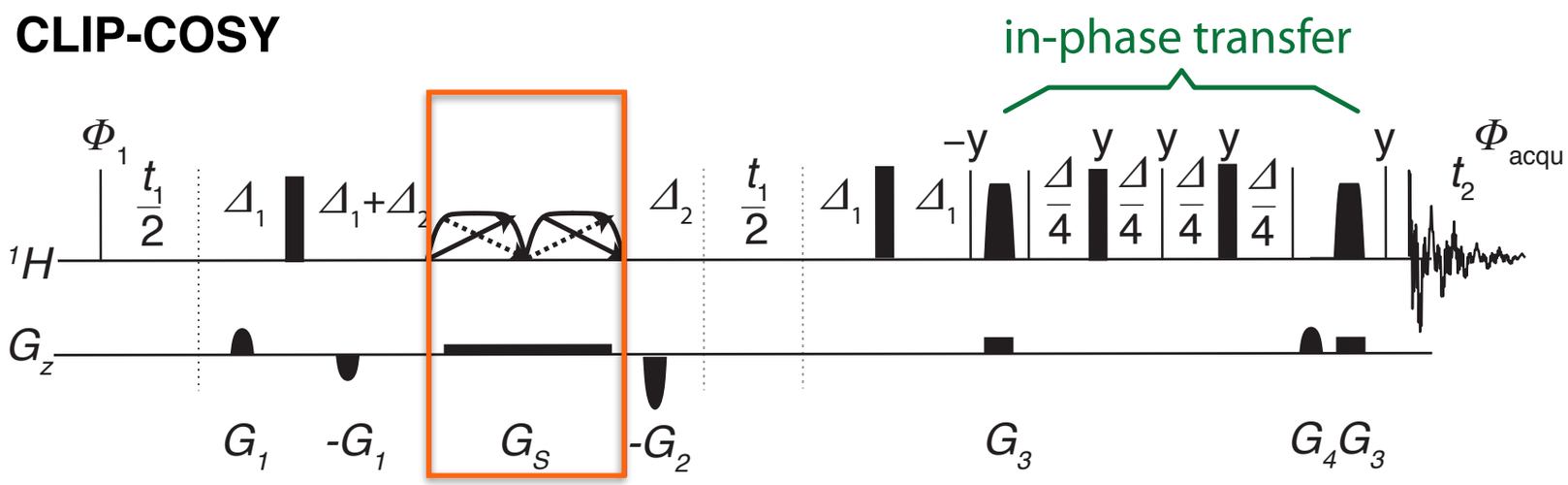


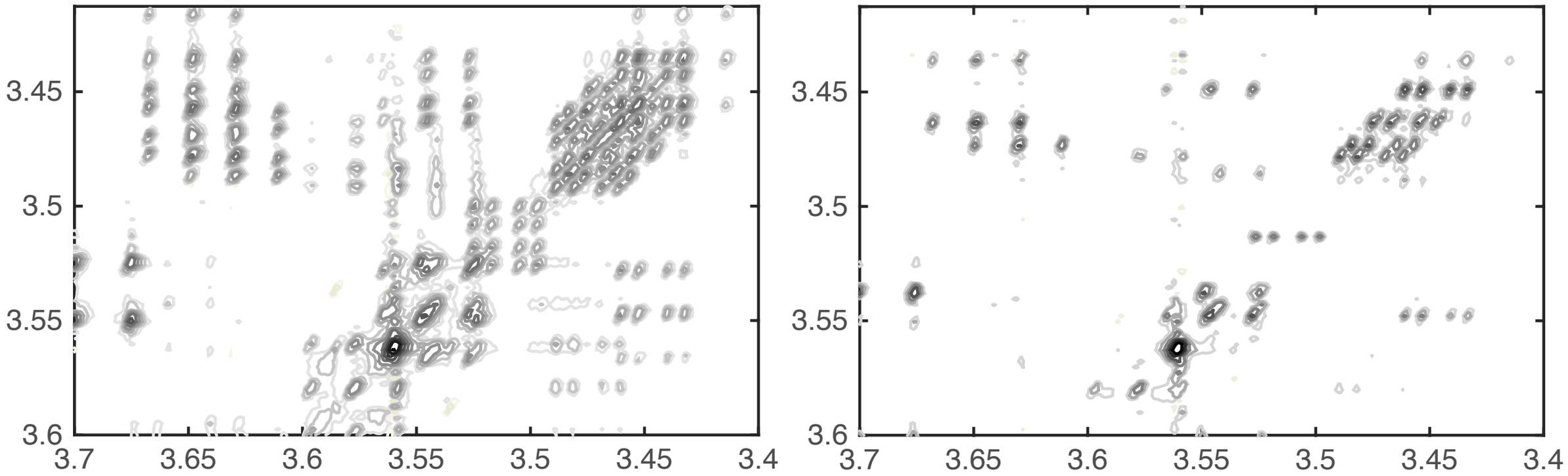




Y. Mitrev, D. Jeannerat, Chem. Commun. 2016

Simplified structure by ***Homodecoupling***

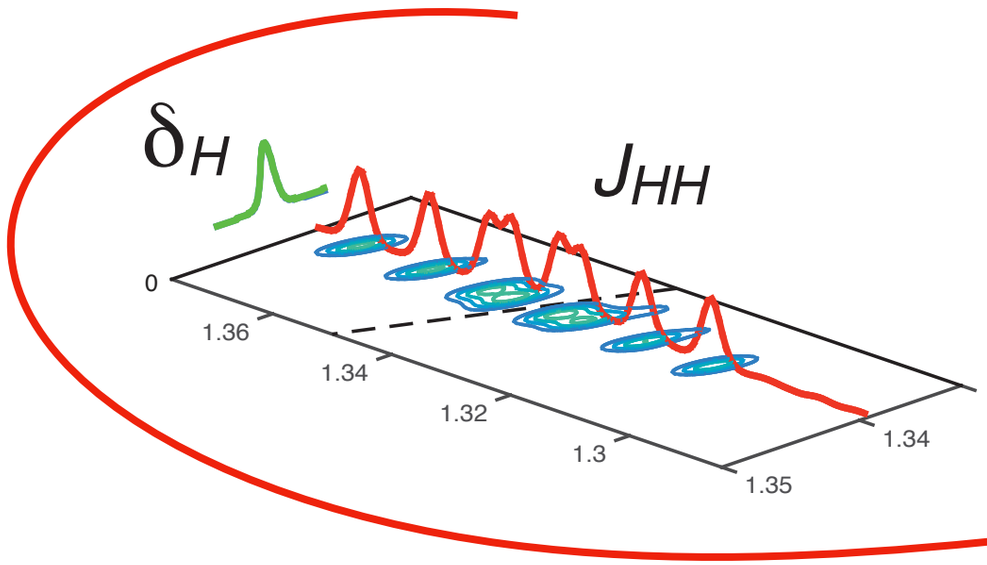




M. R. M. Koos, G. Kummerlowe, L. Kalschnee, C. M. Thiele, B. Luy, Angew. Chem. Int. Ed. 2016, 55.

High-quality spectra

1D ^{1}H, ^{13}C, DEPT
2D COSY
2D HSQC / HMBC …
2D J-Resolved / DIAG



High-quality spectra

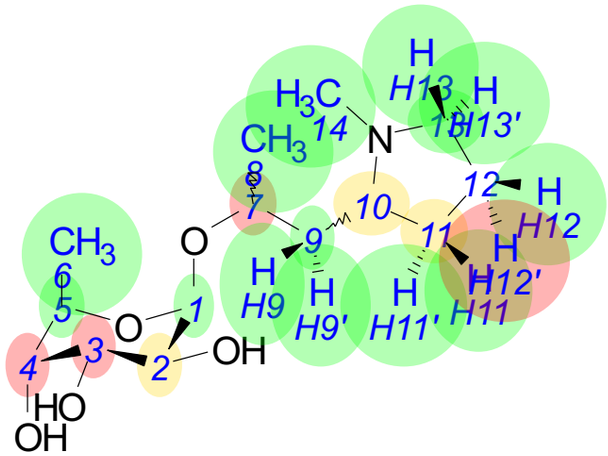
1D ^{1}H, ^{13}C, DEPT
2D COSY
2D HSQC / HMBC …
2D J-Resolved / DIAG

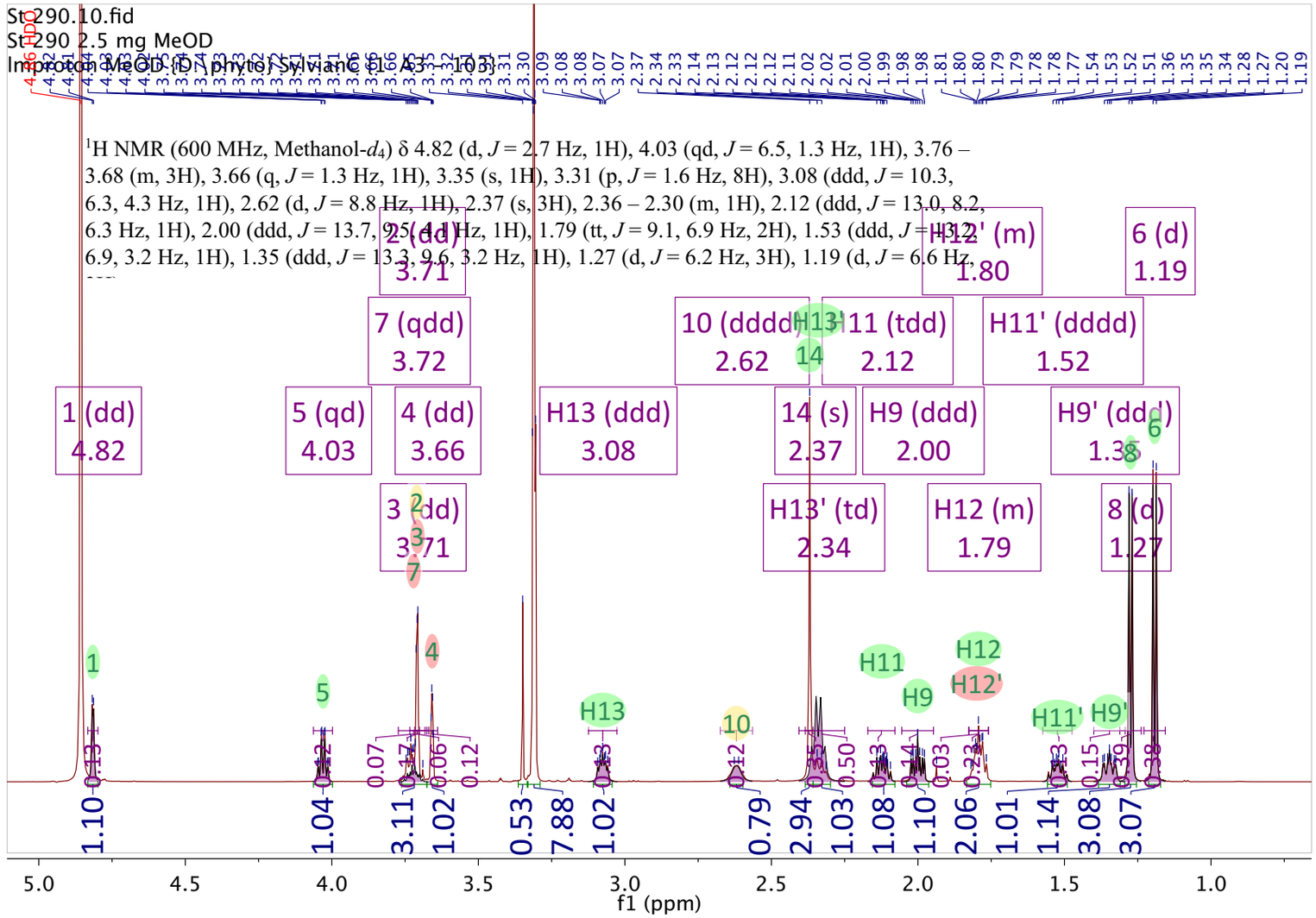
Extract information

Chemical shifts
Scalar couplings
2D correlations
…

Share information

Spectrometer
NMR technician
Chemist
Supervisor
Editor
Reviewer
Publisher
Reader / user





High-quality spectra

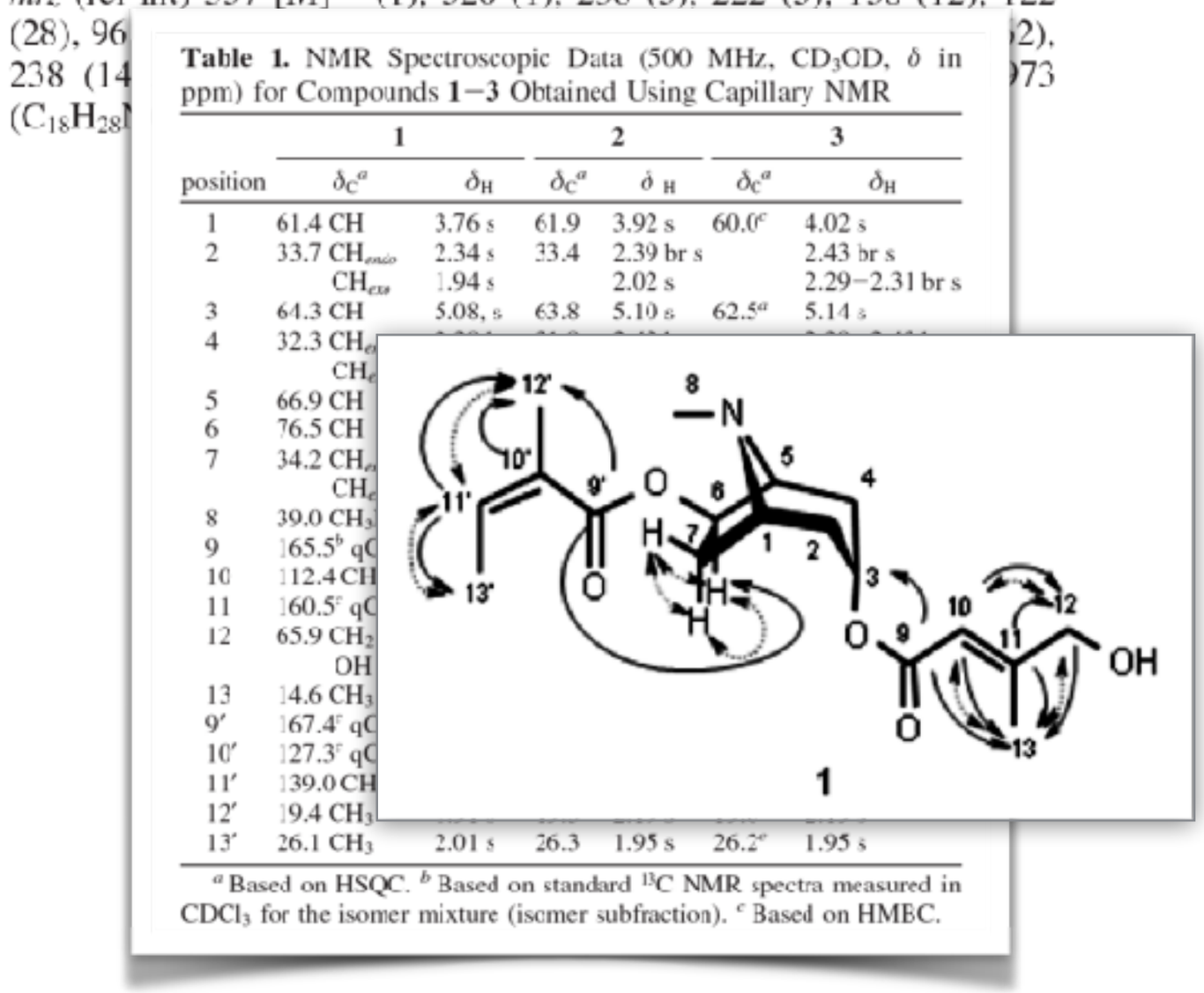
1D ^{1}H, ^{13}C, DEPT
2D COSY
2D HSQC / HMBC …
2D J-Resolved / DIAG

Extract information

Chemical shifts
Scalar couplings
2D correlations
…

Share information

Spectrometer
NMR technician
Chemist
Supervisor
Editor
Reviewer
Publisher
Reader / user



3α-(*E*)-4-Hydroxysenecioyloxy-6*β*-angeloyloxytropane (1): colorless oil; $[\alpha]_D^{25}$ −6.25 (MeOH, *c* 0.04); UV (MeOH) λ_{max} (log ε) 220 nm (2.6); ^{1}H NMR and ^{13}C NMR, see Table 1; RI_{PT} = 2492.4; EIMS *m/z* (rel int) 337 $[M]^{+\cdot}$ (1), 320 (1), 238 (3), 222 (5), 138 (12), 122 (28), 96 …2), 238 (14 …973 ($C_{18}H_{28}$…

Table 1. NMR Spectroscopic Data (500 MHz, CD_3OD, δ in ppm) for Compounds **1**−**3** Obtained Using Capillary NMR

	1		2		3	
position	δ_C[a]	δ_H	δ_C[a]	δ_H	δ_C[a]	δ_H
1	61.4 CH	3.76 s	61.9	3.92 s	60.0[c]	4.02 s
2	33.7 CH_{endo}	2.34 s	33.4	2.39 br s		2.43 br s
	CH_{exo}	1.94 s		2.02 s		2.29−2.31 br s
3	64.3 CH	5.08, s	63.8	5.10 s	62.5[a]	5.14 s
4	32.3 CH_e					
	CH_e					
5	66.9 CH					
6	76.5 CH					
7	34.2 CH_a					
	CH_e					
8	39.0 CH_3					
9	165.5[b] qC					
10	112.4 CH					
11	160.5[c] qC					
12	65.9 CH_2					
	OH					
13	14.6 CH_3					
9′	167.4[c] qC					
10′	127.3[c] qC					
11′	139.0 CH					
12′	19.4 CH_3					
13′	26.1 CH_3	2.01 s	26.3	1.95 s	26.2[c]	1.95 s

[a] Based on HSQC. [b] Based on standard ^{13}C NMR spectra measured in $CDCl_3$ for the isomer mixture (iscmer subfraction). [c] Based on HMBC.

1

Jeannerat, D., Human- and computer-accessible 2D correlation data for a more reliable structure determination of organic compounds. Future roles of researchers, software developers, spectrometer managers, journal editors, reviewers, publisher and database managers toward artificial-intelligence analysis of NMR spectra. *Magn. Reson. Chem.* **2017,** *55* (1), 7-14.

The NMReDATA Initiative

nmredata.org

Academic partners:

Julien Wist[1,§], Jean-Marc Nuzillard[2], Nils E. Schloerer[3], Stefan Kuhn[3], Marion Pupier[4], Mate Erdelyi[5], Christoph Steinbeck[6], Antony J. Williams[9,&], Craig Butts[10], Bozhana Mikhova[11,*], Damien Jeannerat[4,§]

Industrial partners:

Wolfgang Robien

Kessler Pavel[#], Fabrice Moriaud,[#] Mikhail Elyashberg[%], Dimitris Argyropoulos[%], Manuel Pérez[&,§]

Publishing partner:

Patrick Giraudeau[7,§], Roberto R. Gil[8,@], Gary Martin[‡,@], Paul Trevorrow[£]

[1] **University of Valle**, Cali, Colombia
[2] CNRS and **University of Reims-Champagne-Ardenne**, Reims, France
[3] IDNMR, **University of Cologne**, Cologne, Germany
[4] Department of organic chemistry, **University of Geneva**, Geneva, Switzerland
[5] Department of Chemistry - BMC, **University of Uppsala**, Sweden
[6] Cheminformatics and Chemometrics, **Friedrich-Schiller-University Jena**, Germany
[7] CEISAM, **University of Nantes**, Nantes, France
[8] Department of Chemistry, **Carnegie Mellon University**, Pittsburgh, USA
[9] National Center for Computational Toxicology, **EPA**, USA
[10] **University of Bristol**, UK
[11] Institute of organic chemistry, **Bulgarian academy of sciences**, Bulgaria

[#] **Bruker BioSpin GmbH**, Rheinstetten, Germany
[%] **ACD/Labs**, Toronto, Canada
[&] **Mestrelab Research**, Santiago de Compostela, Spain
[‡] **Merck and co**. New-Jersey, USA

Magnetic Resonance in Chemistry, Wiley, Chichester, UK
[@] Coeditors in Chief
[*] Member of the *Editorial board*
[§] Member of the *Associate board*
[&] Member of the *Advisory board*
[£] Executive journal editor

Follow the progress of the initiative on

www.nmredata.org

POSTER 376

NMR record

Spectra

1D ^{1}H

Chemical shifts, couplings, integrals

1D ^{13}C

Chemical shifts, signals intensities

COSY/NOESY

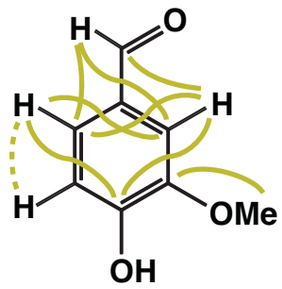
list of crosspeaks

HSQC/HMBC

list of correlations

.sdf file

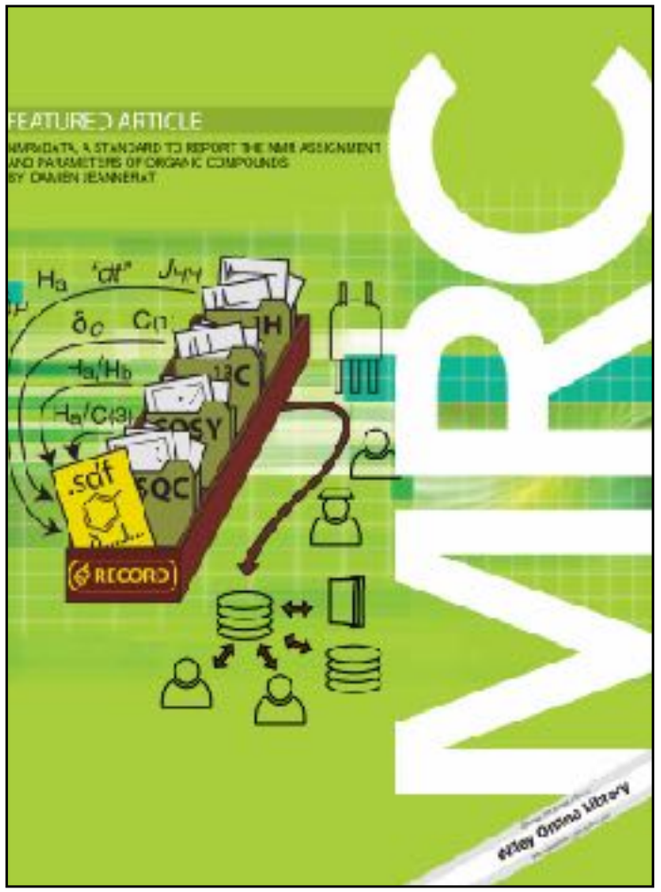
Structure



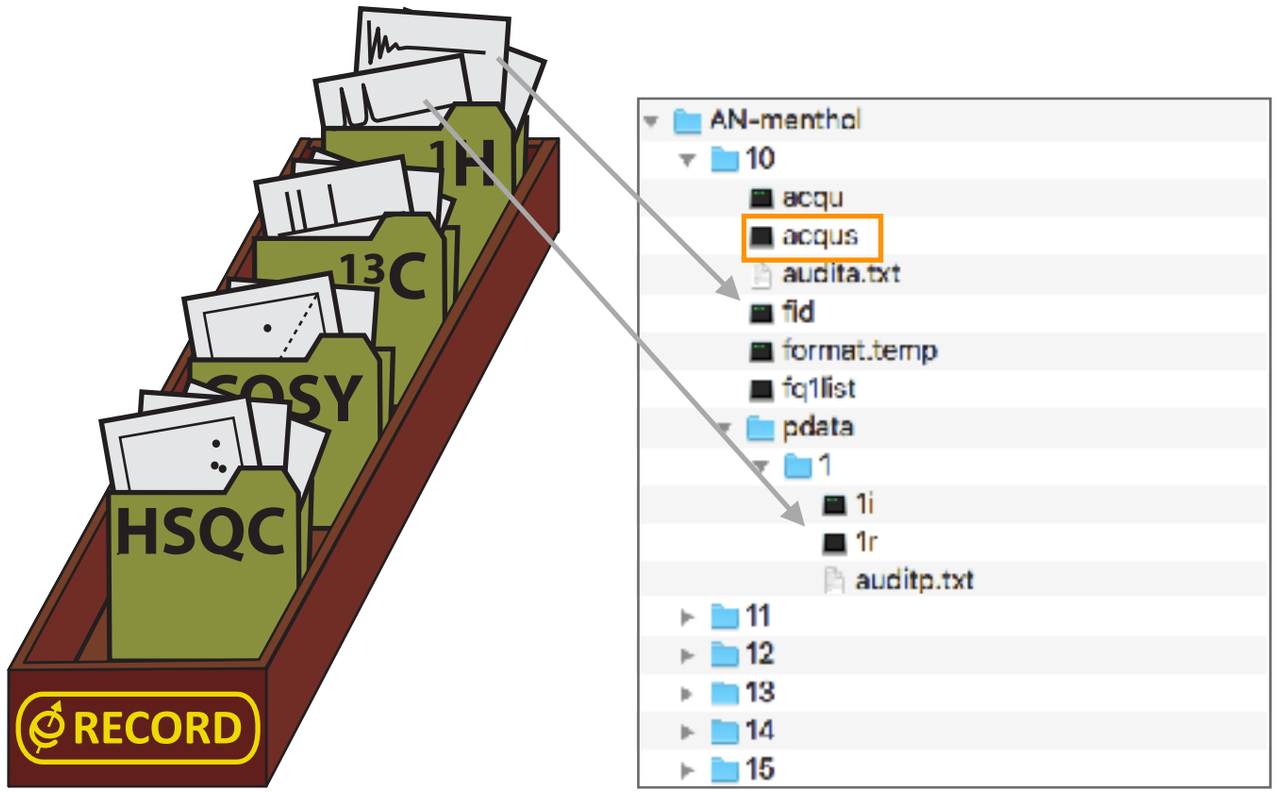
Assigned

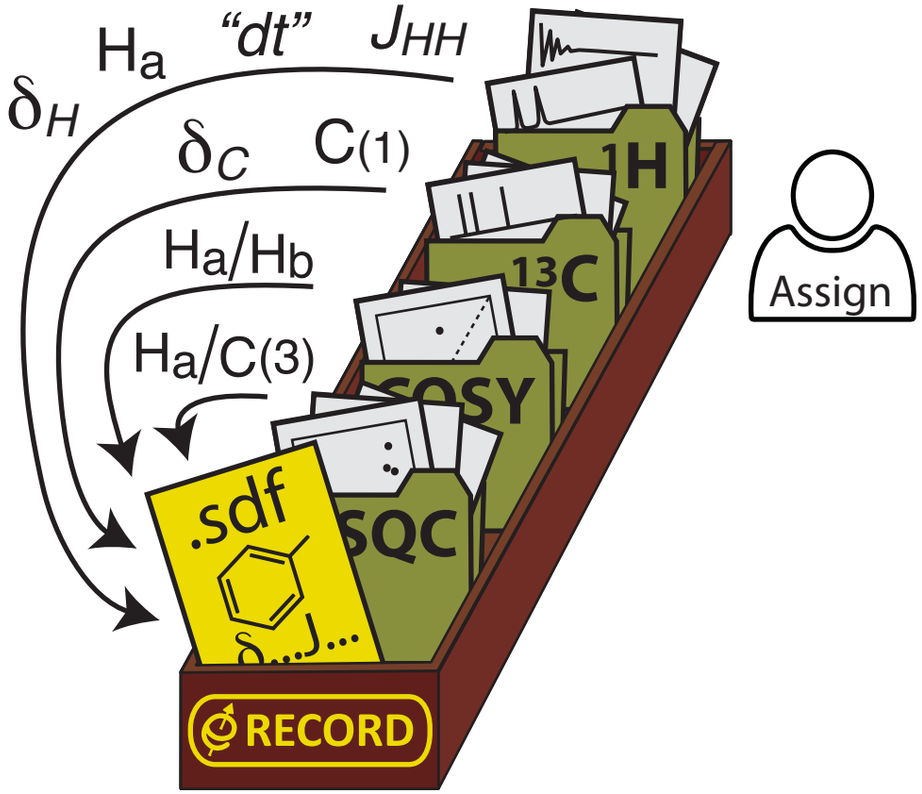
NMReDATA

(see details below)



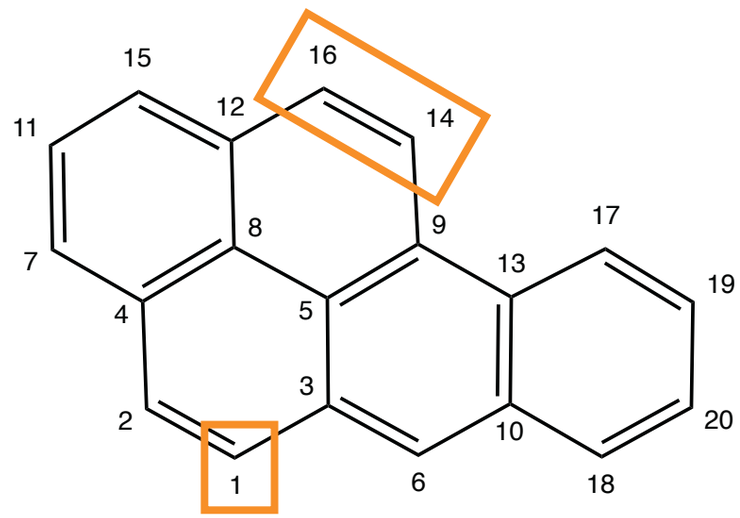
1. Pupier, M.; Nuzillard, J.-M.; Wist, J.; Schlörer, N. E.; Kuhn, S.; Erdelyi, M.; Steinbeck, C.; Williams, A. J.; Butts, C.; Claridge, T. D. W.; Mikhova, B.; Robien, W.; Dashti, H.; Eghbalnia, H. R.; Farès, C.; Adam, C.; Kessler, P.; Moriaud, F.; Elyashberg, M.; Argyropoulos, D.; Pérez, M.; Giraudeau, P.; Gil, R. R.; Trevorrow, P.; Jeannerat, D., NMReDATA, a standard to report the NMR assignment and parameters of organic compounds. *Magn. Reson. in Chem.* **2018**.
DOI: 10.1002/mrc.4737


1H
13C
COSY
HSQC
RECORD
AN-menthol
10
acqu
acqus
audita.txt
fid
format.temp
fq1list
pdata
1
1i
1r
auditp.txt
11
12
13
14
15


Ha
"dt"
JHH
δH
δC
C(1)
Ha/Hb
Ha/C(3)
1H
13C
COSY
SQC
.sdf
RECORD
Assign

.mol

```
benzo(a)pyrene
demo of .sdf file containing NMReDATA
test_generationV1 1
20 24  0  0  0  0  0  0  0  0999 V2000
   -1.6583    2.2334    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.6633    3.1556    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.3753    0.8191    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.7234    2.7603    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.0000    0.3848    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
 ...
    2.6960   -0.4398    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.5264   -3.3746    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.1687   -2.4653    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.5724   -4.2723    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.9104   -3.8155    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  1  2  2  0  0  0
  1  3  1  0  0  0
  2  4  1  0  0  0
  3  5  1  0  0  0
  ...
 13 17  1  0  0  0
 14 16  2  0  0  0
 17 19  2  0  0  0
 18 20  2  0  0  0
 19 20  1  0  0  0
M  END
```



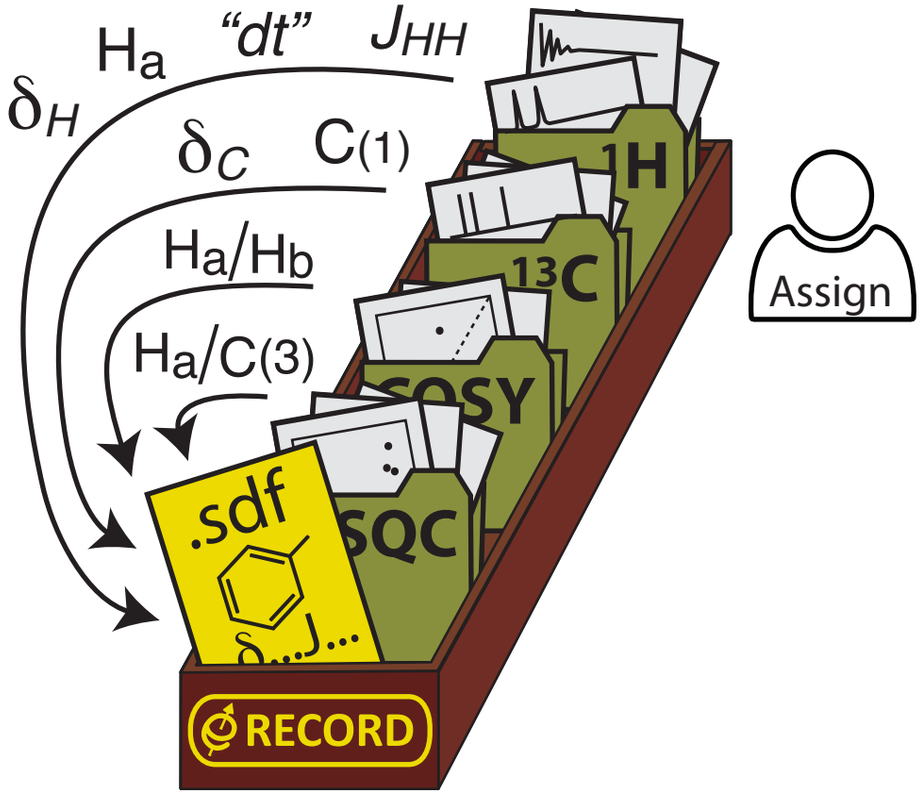
.sdf

Structure Data Format

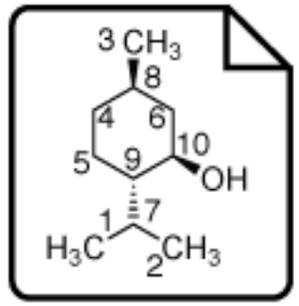
```
>  <NMREDATA_SOLVENT>
cdcl3

>  <NMREDATA_TEMPERATURE>
298.15
```

```
M  ZZC  13 1ax
M  ZZC  14 2ax
M  ZZC  15 2eq
M  ZZC  16 5ax
M  ZZC  17 5eq
M  END
>  <NMREDATA_VERSION>
1.1\

>  <NMREDATA_ID>
Doi=10.5281/zenodo.1146869
Record=http://zenodo.org/record/1146869/files/sample1.zip

>  <NMREDATA_SOLVENT>
CDCl3\

>  <NMREDATA_LEVEL>
0\

>  <NMREDATA_ASSIGNMENT>
1, 34.5669, 1\
2, 23.1445, 2\
H3, 1.1301, H3\
3, 50.1583, 3\
H4, 3.4302, H4\
4, 71.5891, 4\
5, 45.0568, 5\
H6, 1.4444, H6\
6, 31.6232, 6\
H7, 0.9331, H7\
7, 22.2293, 7\
H12, 1.3536, H8\
```

Tag
Tag name
Tag content



Assigned NMReDATA compound1.nmredata.sdf



NMREDATA_1D_13C

NMREDATA_1D_1H

1.1301, S=ddd, L=H9ax, E=42.3746, J=12.76, 9.90, 3.05,2.72
3.4302, S=dddd, L=H10ax, E=28.9715, J=10.90,9.90,4.80,4.50
1.4444, S=ddqdd, L=H8ax, E=27.4764, J=12.00,12.00,6.58,4.00,3.00
...

...

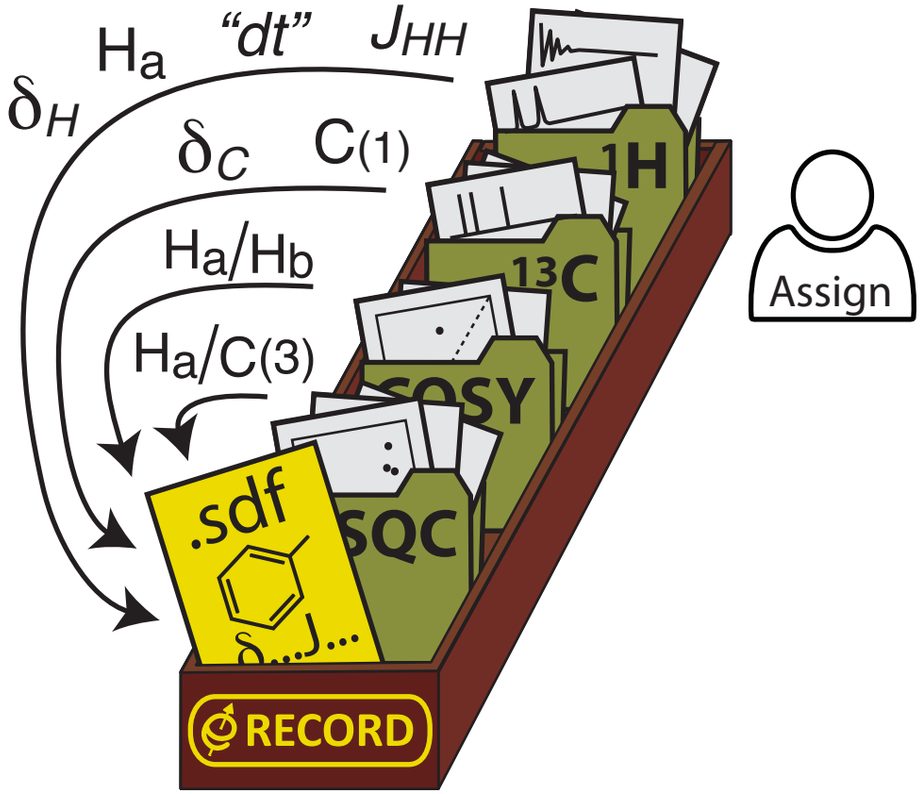
NMREDATA_2D_13C_NJ_1H

NMREDATA_2D_13C_1J_1H

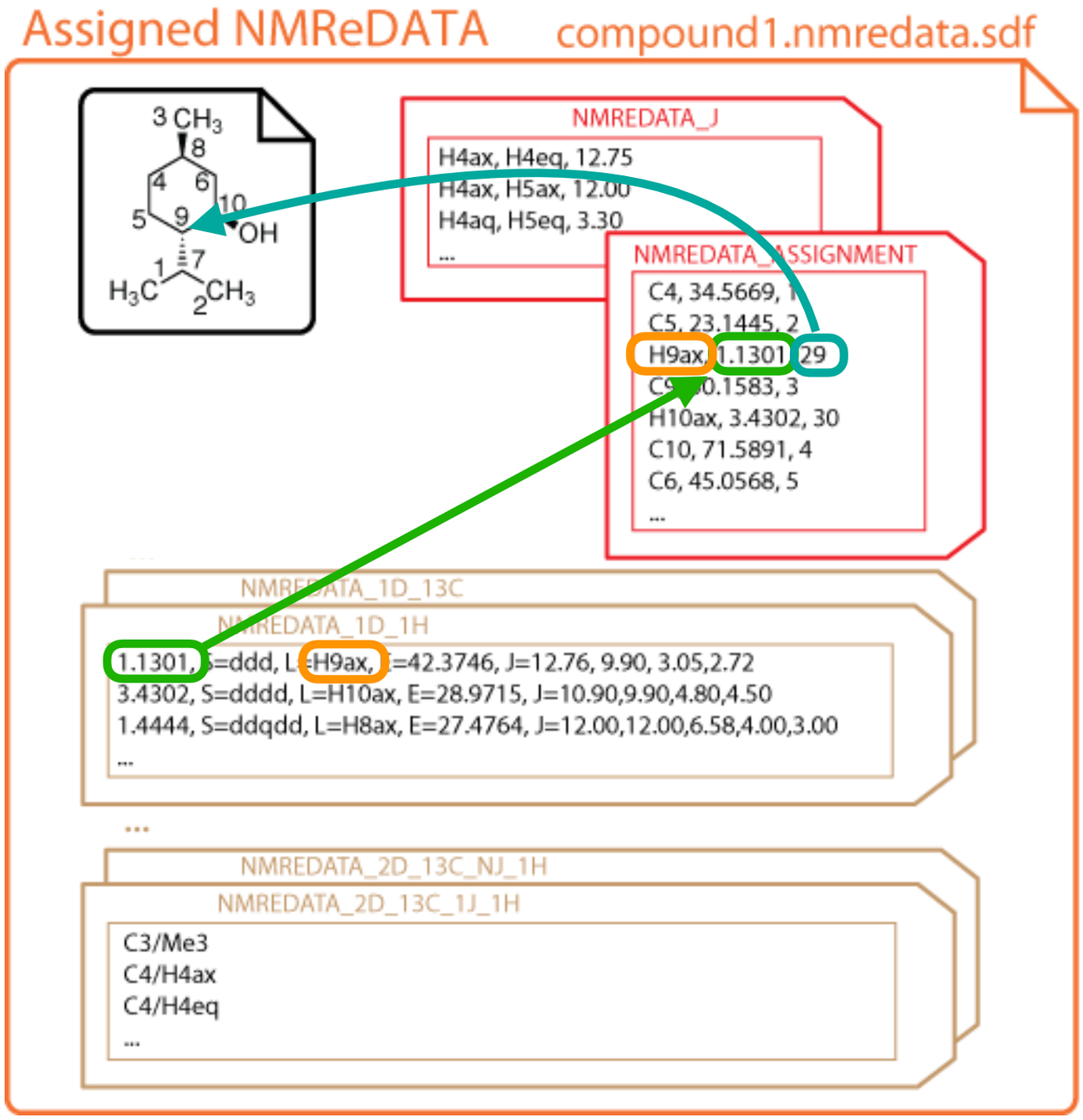
C3/Me3
C4/H4ax
C4/H4eq
...

```
>  <NMREDATA_1D_1H>
Larmor=500.133088507\
Pulseprogram=zg30
Spectrum_Location=file:AN-menthol/10/pdata/1/\
1.1301, S=dddd, L=H3, E=42.3746, J=12.76,9.90,3.05,2.72\
3.4302, S=dddd, L=H4, E=28.9715, J=10.90,9.90,4.80,4.30\
1.4444, S=ddtdd, L=H6, E=27.4764, J=12.00,12.00,6.58,4.00,3.00\
2.1895, S=ddd, L=H9, E=42.6060, J=7.02,6.90,2.72\
…

>  <NMREDATA_1D_13C>
Larmor=125.770363831\
Pulseprogram=dept135 ;optional in V1\
Spectrum_Location=file:AN-menthol/12/pdata/1/\
…

>  <NMREDATA_2D_1H_NJ_1H>
Larmor=500.13\
CorrType=COSY\
Pulseprogram=cosygpmfph2
Spectrum_Location=file:dj_menthol/21/pdata/1/\
H4/H3\
H9/H3\
H3/H4\
H12/H4\
H5ax/H4\
H5eq/H4\
H7/H6\
```

```
>  <NMREDATA_1D_1H>
Larmor=500.133088507\
Pulseprogram=zg30
Spectrum_Location=file:AN-menthol/10/pdata/1/\
1.1301, S=dddd, L=H3, E=42.3746, J=12.76,9.90,3.05,2.72\
3.4302, S=dddd, L=H4, E=28.9715, J=10.90,9.90,4.80,4.30\
1.4444, S=ddtdd, L=H6, E=27.4764, J=12.00,12.00,6.58,4.00,3.00\
2.1895, S=ddd, L=H9, E=42.6060, J=7.02,6.90,2.72\
…

>  <NMREDATA_1D_13C>
Larmor=125.770363831\
Pulseprogram=dept135 ;optional in V1\
Spectrum_Location=file:AN-menthol/12/pdata/1/\
…

>  <NMREDATA_2D_1H_NJ_1H>
Larmor=500.13\
CorrType=COSY\
Pulseprogram=cosygpmfph2
Spectrum_Location=file:dj_menthol/21/pdata/1/\
H4/H3\
H9/H3\
H3/H4\
H12/H4\
H5ax/H4\
H5eq/H4\
H7/H6\
```



Desired redundance and complementarity



Label / δ / Atom number

```
>  <NMREDATA_ASSIGNMENT>
1, 34.5669, 1\
2, 23.1445, 2\
H3, 1.1301, H3\
3, 50.1583, 3\
H4, 3.4302, H4\
4, 71.5891, 4\
5, 45.0568, 5\
H6, 1.4444, H6\
6, 31.6232, 6\
H7, 0.9331, H7\
7, 22.2293, 7\
H12, 1.3536, H8\
H9, 2.1895, H9\
9, 25.8422, 9\
H10, 0.8311, H10\
10, 16.1017, 10\
H11, 0.9493, H11\
11, 20.9880, 11\
H1eq, 1.6822, 12\
H1ax, 0.8630, 13\
H2ax, 0.9933, 14\
H2eq, 1.6293, 15\
H5ax, 0.9535, 16\
H5eq, 1.9844, 17\
```

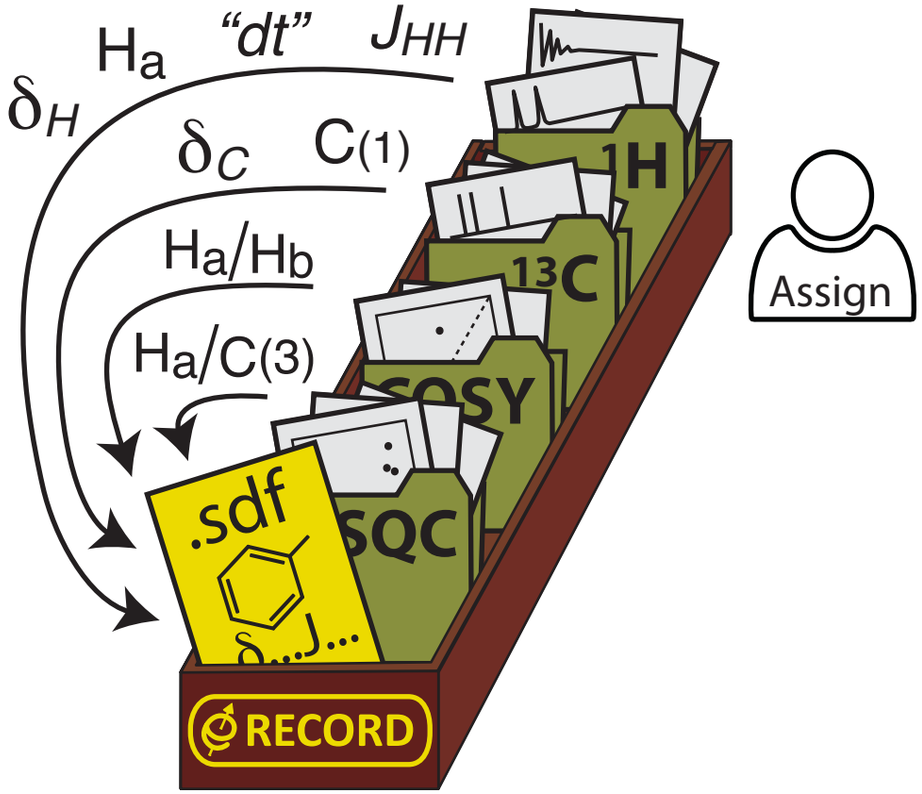
When H atoms are implicit add “H”…

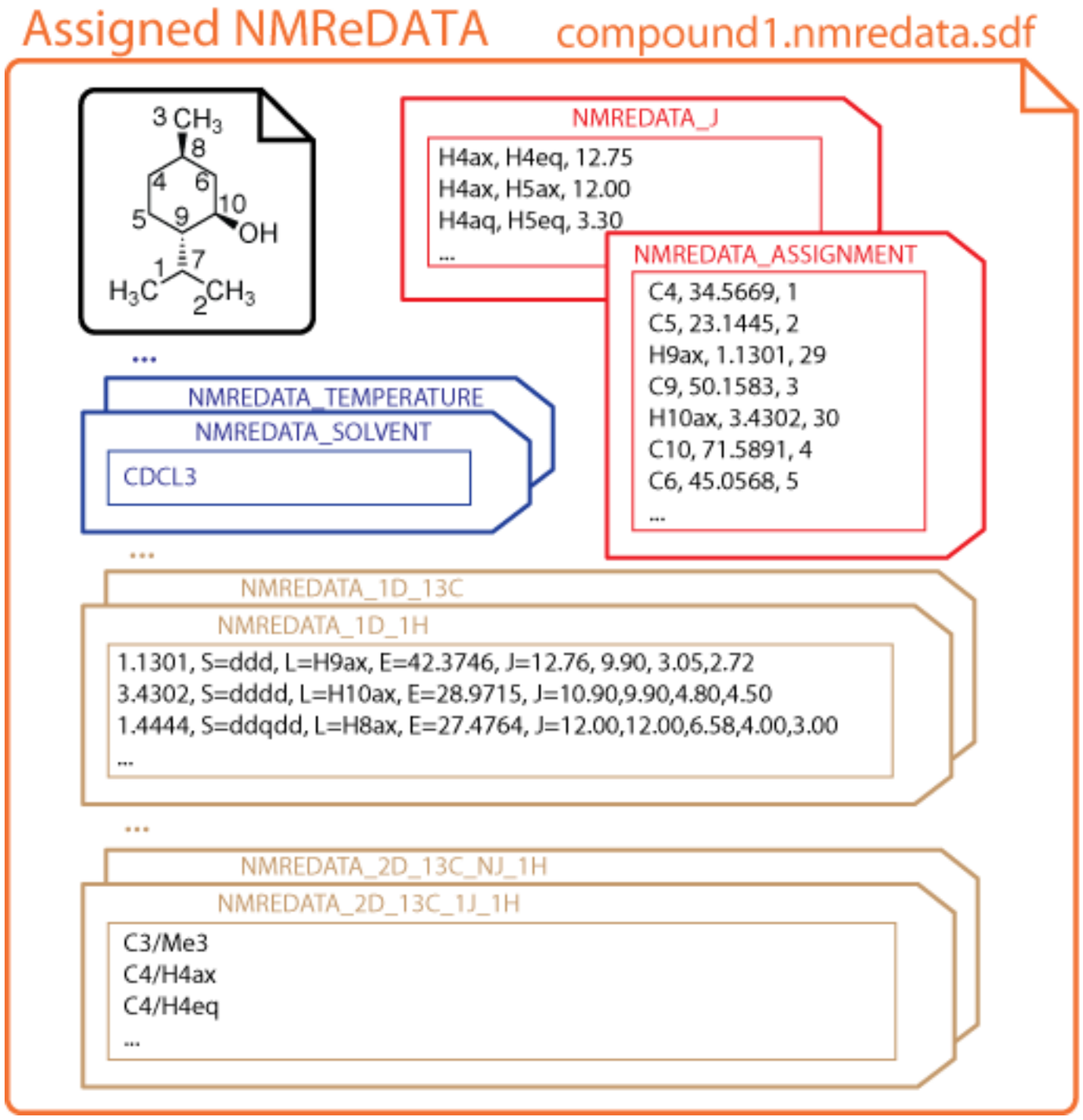
Label / δ / Atom number

```
>  <NMREDATA_ASSIGNMENT>
1, 34.5669, 1\
2, 23.1445, 2\
H3, 1.1301, H3\
3, 50.1583, 3\
H4, 3.4302, H4\
4, 71.5891, 4\
5, 45.0568, 5\
H6, 1.4444, H6\
6, 31.6232, 6\
H7, 0.9331, H7\
7, 22.2293, 7\
H12, 1.3536, H8\
H9, 2.1895, H9\
9, 25.8422, 9\
H10, 0.8311, H10\
10, 16.1017, 10\
H11, 0.9493, H11\
11, 20.9880, 11\
H1eq, 1.6822, 12\
H1ax, 0.8630, 13\
H2ax, 0.9933, 14\
H2eq, 1.6293, 15\
H5ax, 0.9535, 16\
H5eq, 1.9844, 17\
```

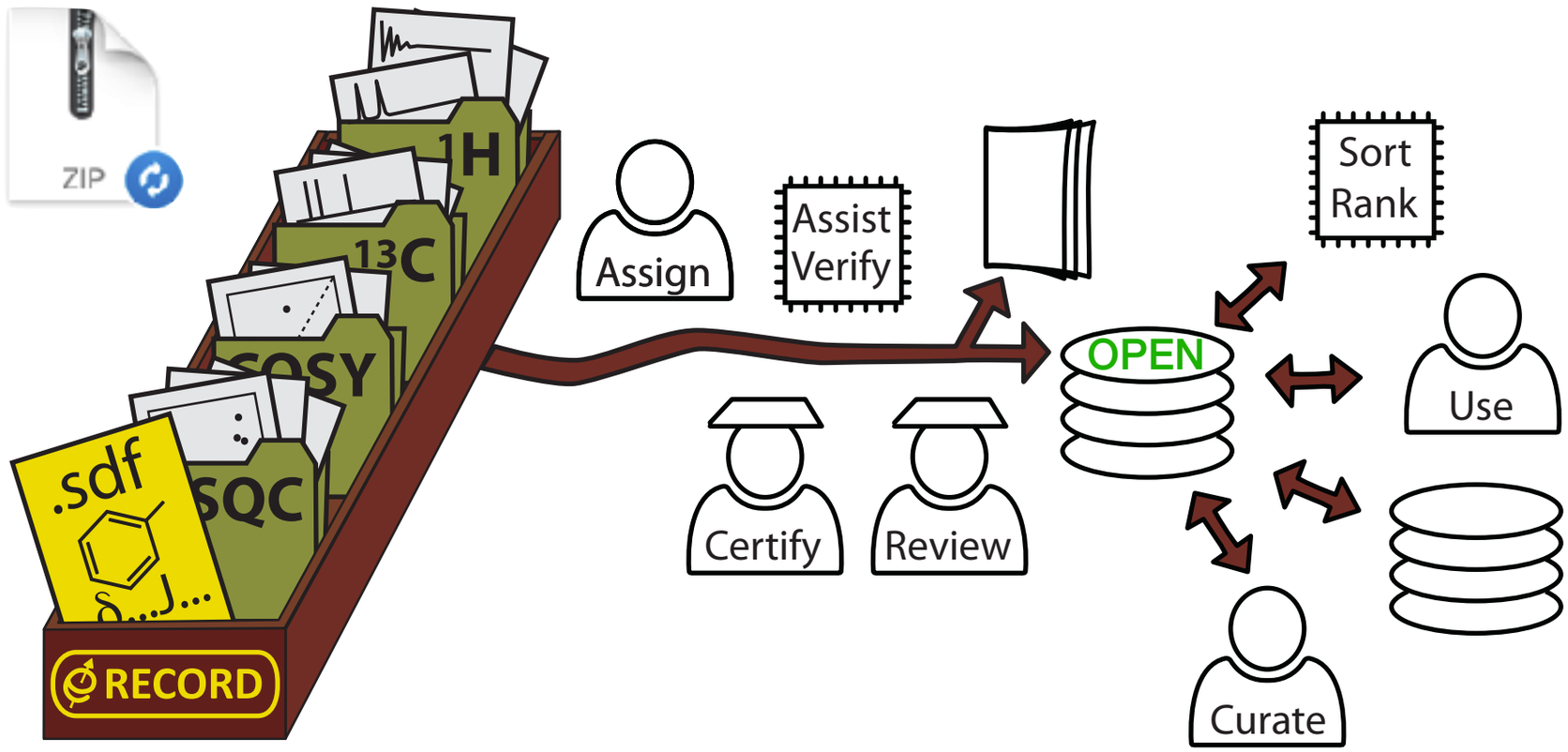
optional

```
>  <NMREDATA_J>
H3, H2ax, 12.8\
H3, H2eq, 3.0\
H3, H4, 9.9\
H3, H9, 2.7\
H4, H12, 4.8\
H4, H5ax, 10.9\
H4, H5eq, 4.5\
H6, H7, 6.6\
H6, H1eq, 3.0\
H6, H1ax, 12.0\
H6, H5ax, 12.0\
H6, H5eq, 4.0\
H9, H10, 7.0\
H9, H11, 7.1\
H1eq, H1ax, 12.8\
H1eq, H2ax, 3.3\
H1eq, H2eq, 3.2\
H1eq, H5eq, 2.2\
H1ax, H2ax, 12.0\
H1ax, H2eq, 3.3\
H2ax, H2eq, 13.0\
H5ax, H5eq, 12.1\
```

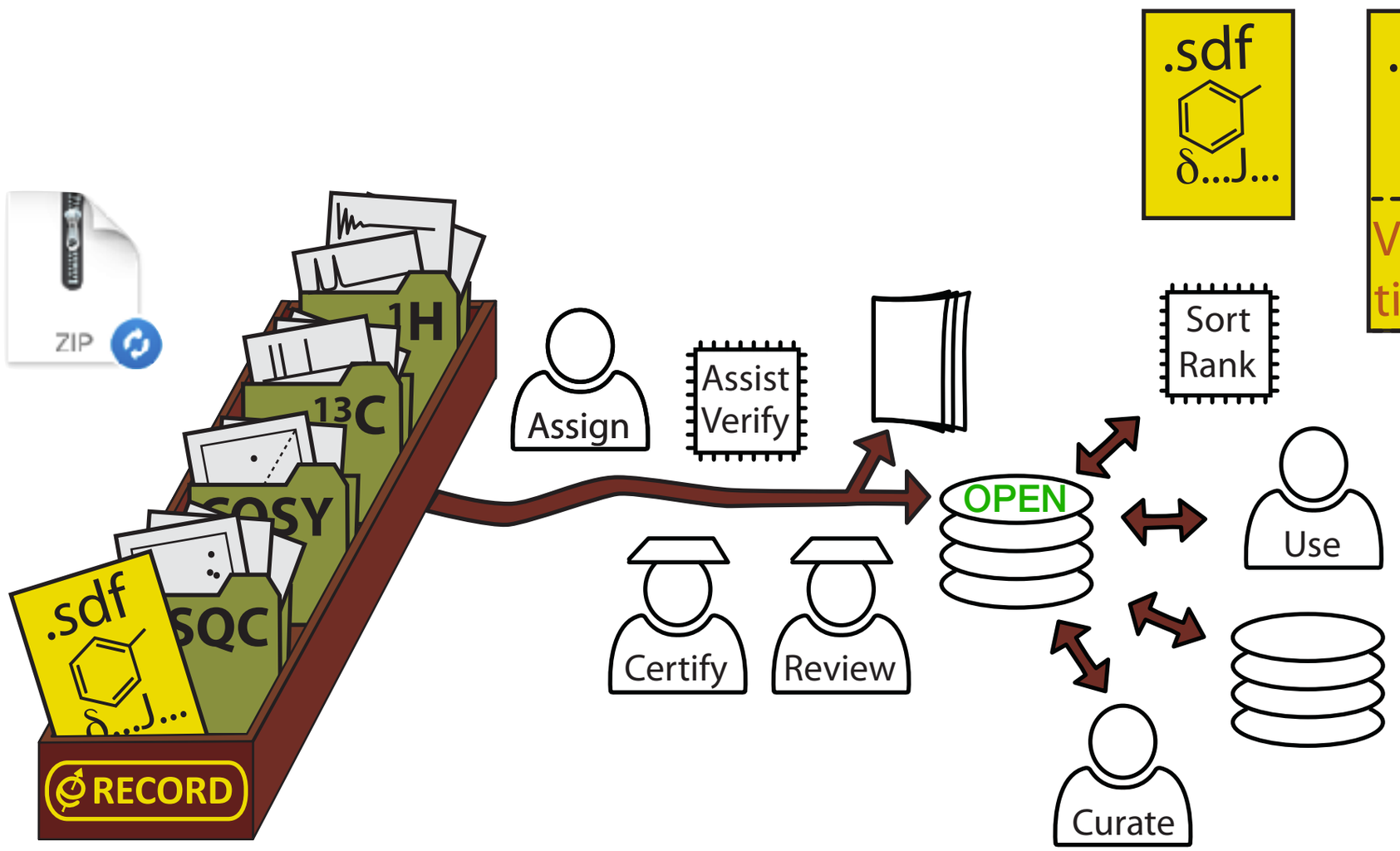

Ha
"dt"
JHH
δH
δC
C(1)
Ha/Hb
Ha/C(3)
1H
13C
COSY
HSQC
.sdf
RECORD
Assign


Assigned NMReDATA
compound1.nmredata.sdf
NMREDATA_J
H4ax, H4eq, 12.75
H4ax, H5ax, 12.00
H4aq, H5eq, 3.30
...
NMREDATA_ASSIGNMENT
C4, 34.5669, 1
C5, 23.1445, 2
H9ax, 1.1301, 29
C9, 50.1583, 3
H10ax, 3.4302, 30
C10, 71.5891, 4
C6, 45.0568, 5
...
NMREDATA_TEMPERATURE
NMREDATA_SOLVENT
CDCL3
NMREDATA_1D_13C
NMREDATA_1D_1H
1.1301, S=ddd, L=H9ax, E=42.3746, J=12.76, 9.90, 3.05,2.72
3.4302, S=dddd, L=H10ax, E=28.9715, J=10.90,9.90,4.80,4.50
1.4444, S=ddqdd, L=H8ax, E=27.4764, J=12.00,12.00,6.58,4.00,3.00
...
NMREDATA_2D_13C_NJ_1H
NMREDATA_2D_13C_1J_1H
C3/Me3
C4/H4ax
C4/H4eq
...

```
M  ZZC  13 1ax
M  ZZC  14 2ax
M  ZZC  15 2eq
M  ZZC  16 5ax
M  ZZC  17 5eq
M  END
>  <NMREDATA_VERSION>
1.1\

>  <NMREDATA_ID>
Doi=10.5281/zenodo.1146869
Record=http://zenodo.org/record/1146869/files/sample1.zip

>  <NMREDATA_SOLVENT>
CDCl3\

>  <NMREDATA_LEVEL>
0\

>  <NMREDATA_ASSIGNMENT>
1, 34.5669, 1\
2, 23.1445, 2\
H3, 1.1301, H3\
3, 50.1583, 3\
H4, 3.4302, H4\
4, 71.5891, 4\
5, 45.0568, 5\
H6, 1.4444, H6\
6, 31.6232, 6\
H7, 0.9331, H7\
7, 22.2293, 7\
H12, 1.3536, H8\
```


ZIP
1H
13C
COSY
.sdf
SQC
RECORD
Assign
Assist
Verify
OPEN
Sort
Rank
Use
Certify
Review
Curate

```
M  ZZC  13 1ax
M  ZZC  14 2ax
M  ZZC  15 2eq
M  ZZC  16 5ax
M  ZZC  17 5eq
M  END
>  <NMREDATA_VERSION>
1.1\

>  <NMREDATA_ID>
Doi=10.5281/zenodo.1146869
Record=http://zenodo.org/record/1146869/files/sample1.zip

>  <NMREDATA_SOLVENT>
CDCl3\

>  <NMREDATA_LEVEL>
0\

>  <NMREDATA_ASSIGNMENT>
1, 34.5669, 1\
2, 23.1445, 2\
H3, 1.1301, H3\
3, 50.1583, 3\
H4, 3.4302, H4\
4, 71.5891, 4\
5, 45.0568, 5\
H6, 1.4444, H6\
6, 31.6232, 6\
H7, 0.9331, H7\
7, 22.2293, 7\
H12, 1.3536, H8\
```

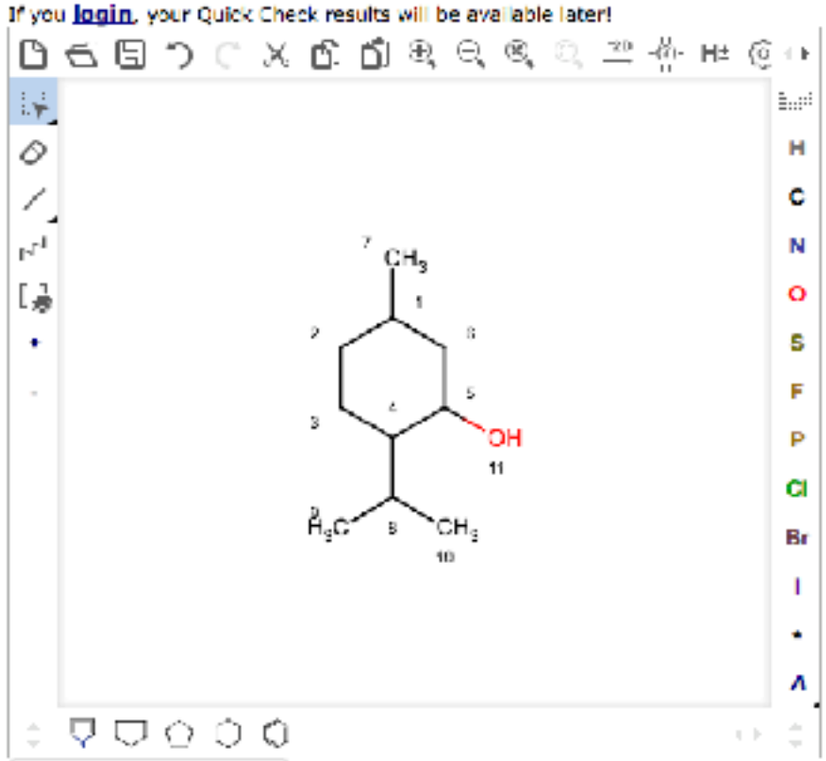

ZIP
1H
13C
COSY
.sdf
RECORD
Assign
Assist
Verify
OPEN
Certify
Review
Curate
Sort
Rank
Use
.sdf
δ...J...
.sdf
δ...J...
Valida-
tion δ

Validation of δ

http://nmrshiftdb.nmr.uni-koeln.de/

NMRShiftDB

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



Import from structure 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		Keep unchanged 3.62
	35.0 Keep unchanged 31.80, diff: 3.20	Keep unchanged 1.44
2	34.80, diff: 5.20	Keep unchanged 1.26
3	Keep unchanged 23.35	Keep unchanged 1.30
4	Keep unchanged 50.25	Keep unchanged 1.12
5	Keep unchanged 71.10	Keep unchanged 3.42
6	Keep unchanged 45.35	Keep unchanged 1.47
7	Keep unchanged 22.25	Keep unchanged 0.93
8	Keep unchanged 25.75	Keep unchanged 2.10
9	Keep unchanged * 18.55	Keep unchanged * 0.88
10	Keep unchanged * 18.55	Keep unchanged * 0.88

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

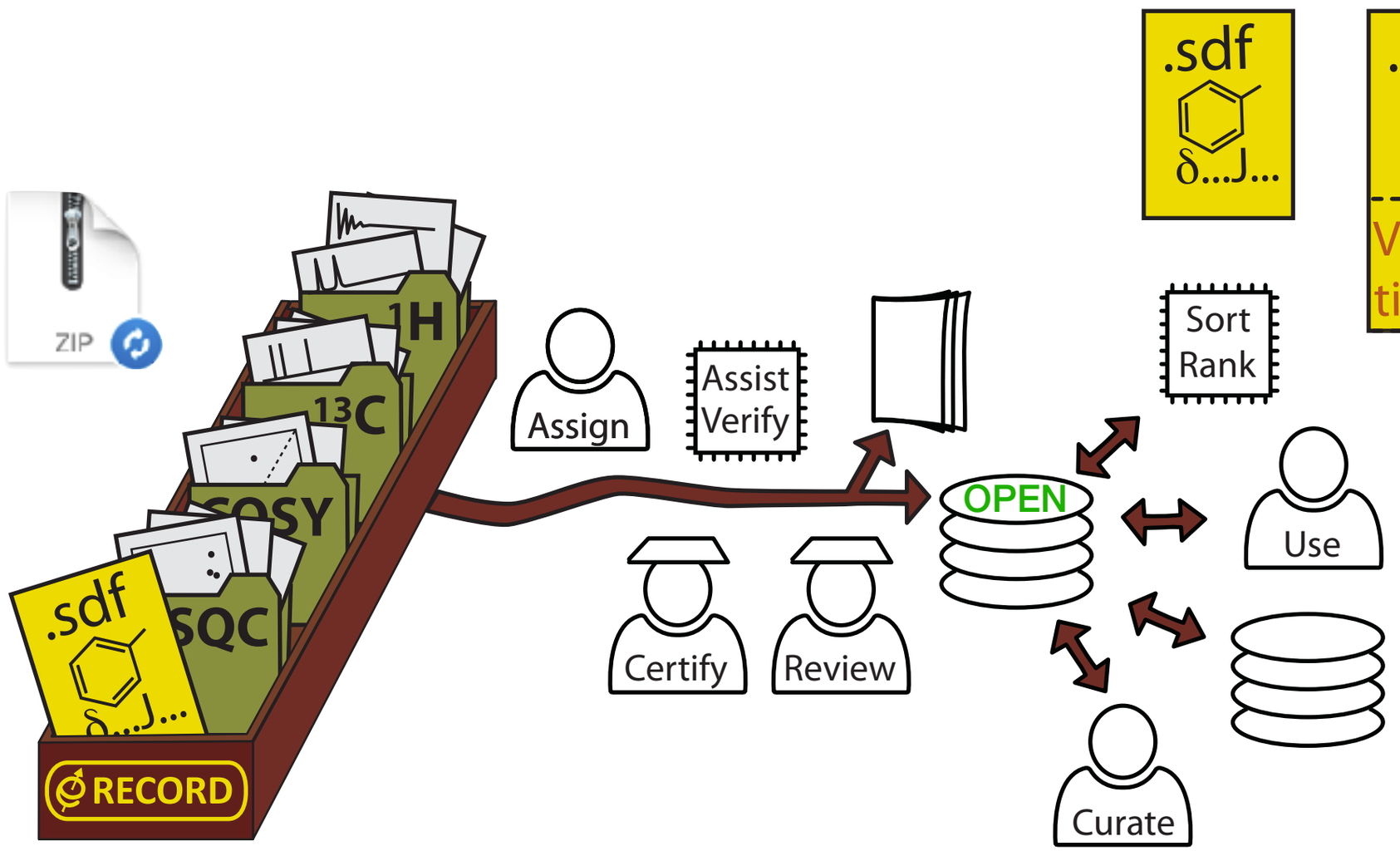
Input list: **Input format**

```
Shifts for auto
assignment, format
like:
56.25
64.10
multiplicity optional
```

Submit ^{1}H

Input list: **Input format**

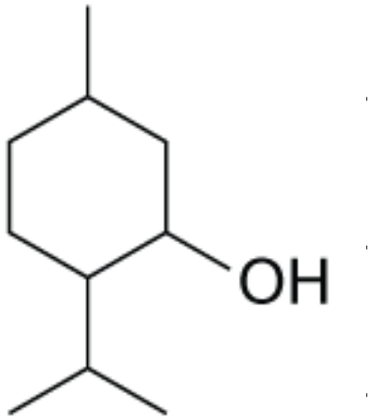
```
Shifts for auto
assignment, format like:
56.2
64.1
Enter diastereotopic pairs
like this:
1.8
-1.6
```

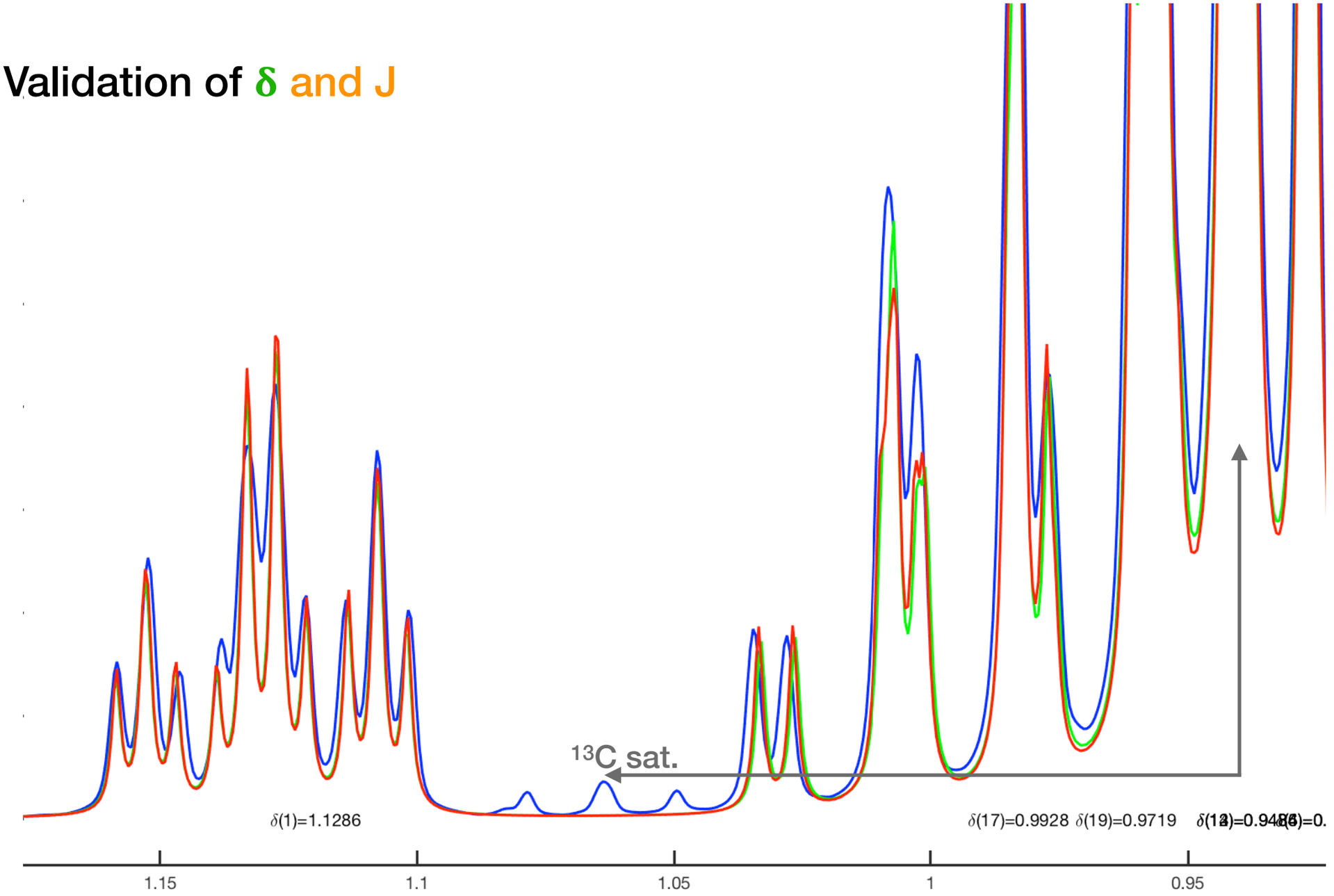

ZIP
1H
13C
COSY
.sdf
RECORD
Assign
Assist
Verify
OPEN
Certify
Review
Curate
Sort
Rank
Use
.sdf
δ...J...
.sdf
δ...J...
Valida-
tion δJ

Validation of δ and J

… with assignment of J, can reproduce 2nd order effects

Refinement + Validation of δ and J



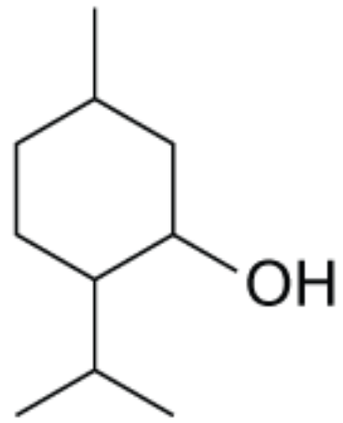


SPINACH : Kuprov, I., Large-scale NMR simulations in liquid state: A tutorial. *Magn. Reson. Chem.* **2017**.

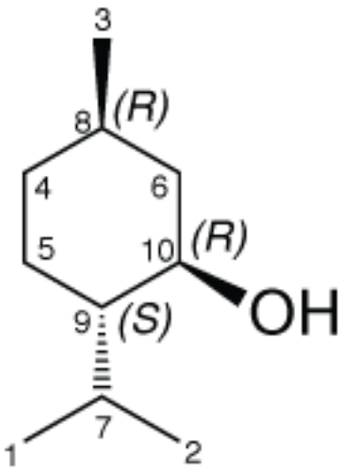
Validation of δ and J

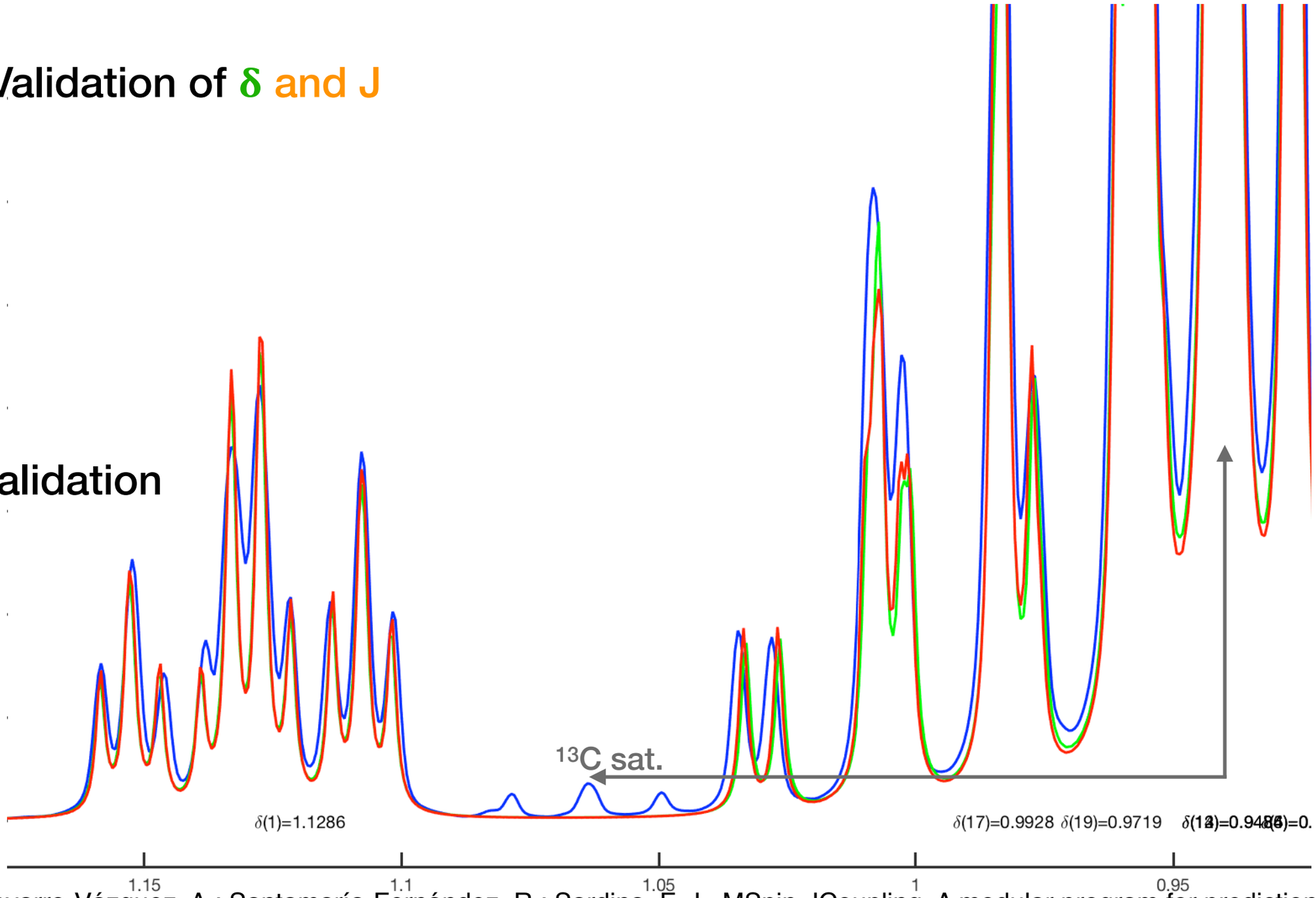
… with assignment of J, can reproduce 2nd order effects

Refinement + Validation of δ and J

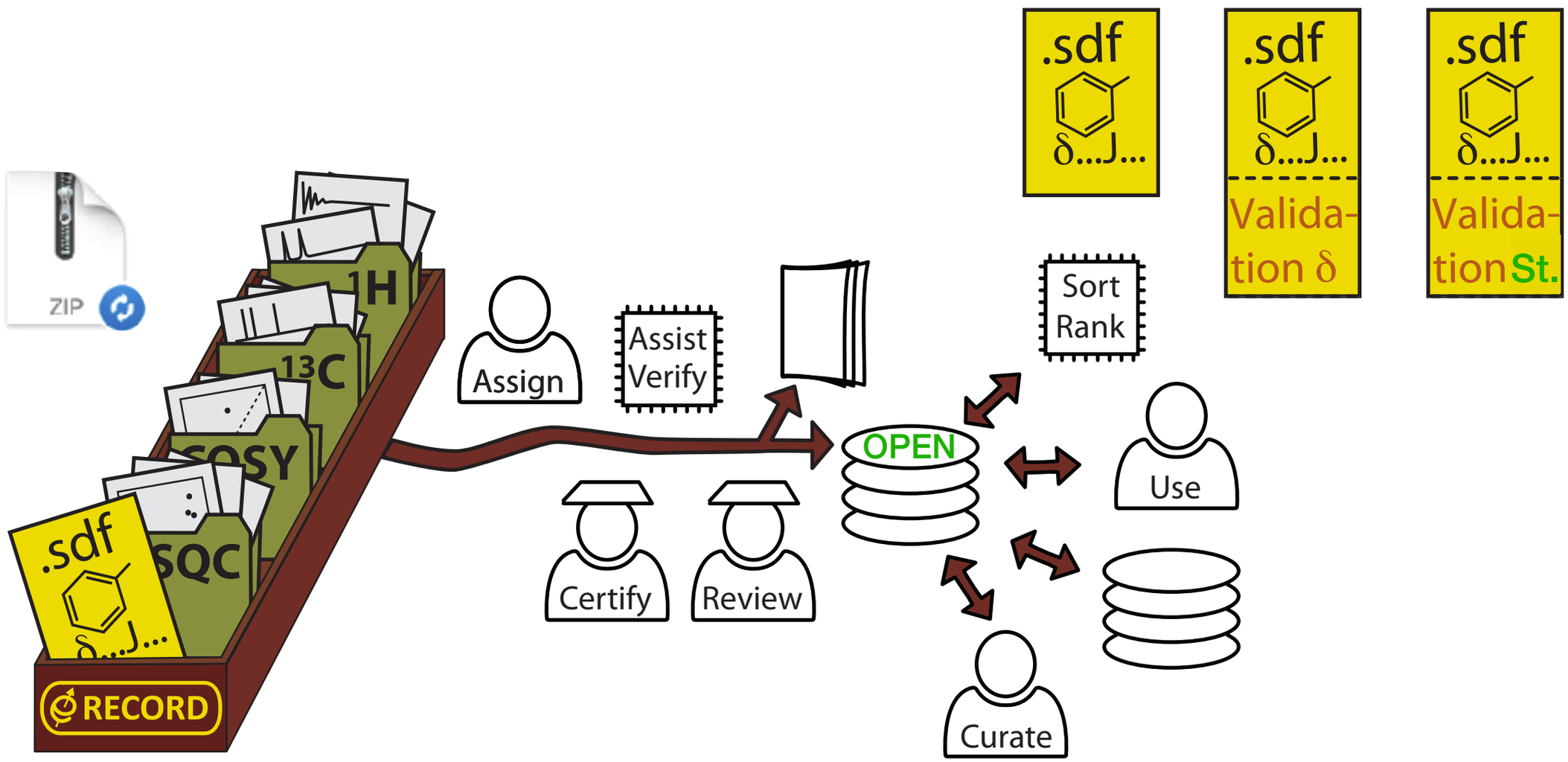


3D structure validation



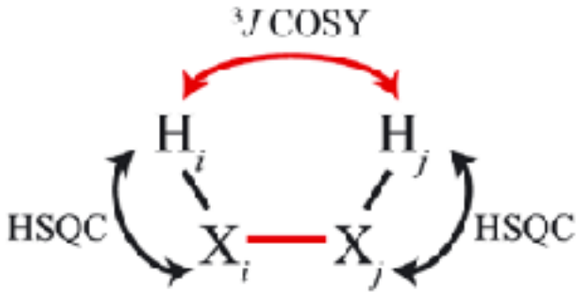


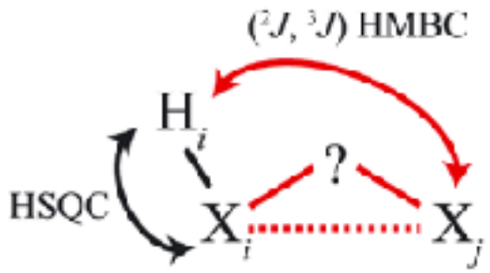
MSpin-JCoupling : Navarro-Vázquez, A.; Santamaría-Fernández, R.; Sardina, F. J., MSpin-JCoupling. A modular program for prediction of scalar couplings and fast implementation of Karplus relationships. *Magn. Reson. Chem.* **2017**.

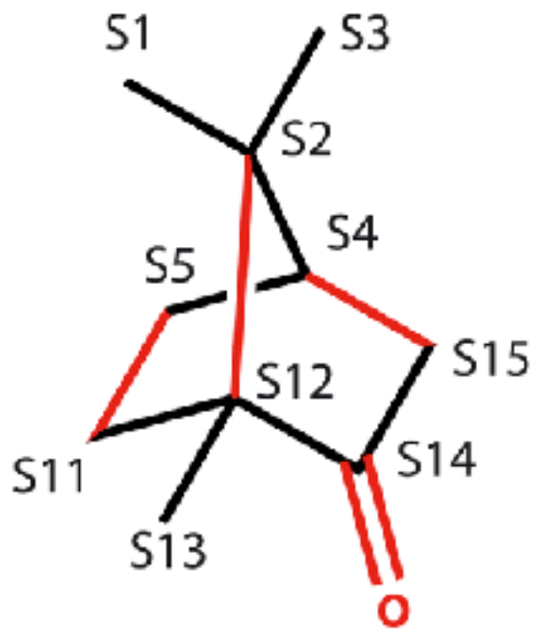

.sdf
δ...J...
.sdf
δ...J...
Valida-
tion δ
.sdf
δ...J...
Valida-
tion St.
ZIP
1H
13C
COSY
.sdf
SQC
RECORD
Assign
Assist
Verify
Sort
Rank
OPEN
Use
Certify
Review
Curate

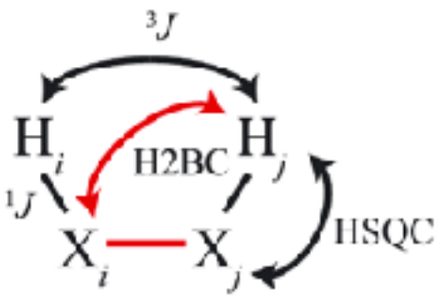
Validation of 2D J correlations using Logic for Structure Determinatin (LSD)

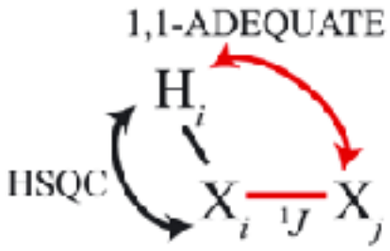
(COSY, HSQC, HMBC, *etc.*)

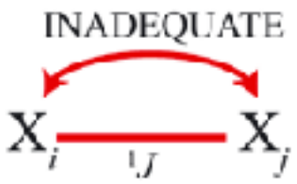




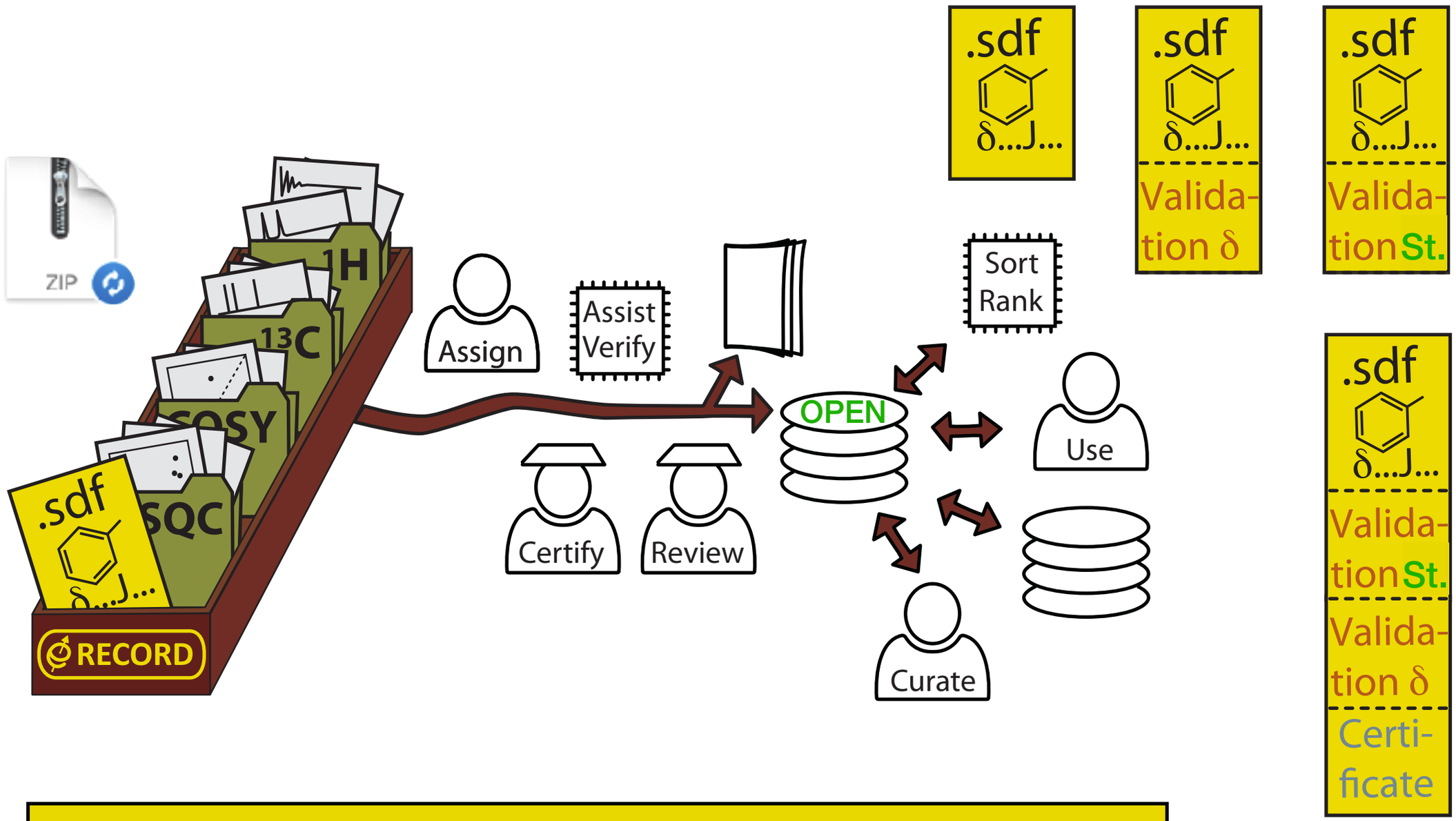








LSD : Nuzillard, J. M.; Plainchont, B., Tutorial for the structure elucidation of small molecules by means of the LSD software. *Magn. Reson. Chem.* **2017**.



.sdf

NMReDATA
MSeDATA - beeing considered
REACeDATA - info. about the origin of the sample
NATSOURCEeDATA - Natural products

Compatible software and web service

Working software and tools

Software Platform	Product/tool	Developer	Operating system	Version	NMReDATA	Supported NMReDATA versions	NMR Record	Examples of output
nmrshiftdb2	QuickCheck	Stefan Kuhn	Web browser	4.1.12	generate/write	1.0 & 1.1	generate	link
Javatools GUI and library	see github	Stefan Kuhn	Any Java-enabled	Pre-alpha	generate/write /validate	1.0 & 1.1	generate	
ACD/Spectrus	Spectrus Processor and above	ACD/Labs	Windows	v. 2017.2	generate/write		generate/write	
Mnova	Mnova script exporting .mnova files	Damien Jeannerat	Any system running Mnova	V.1.1 (see below)	generate		generate (When spectra are available)	NMR records

Julien Wist
Niels Schlörer
Stefan Kuhn
Luc Patiny

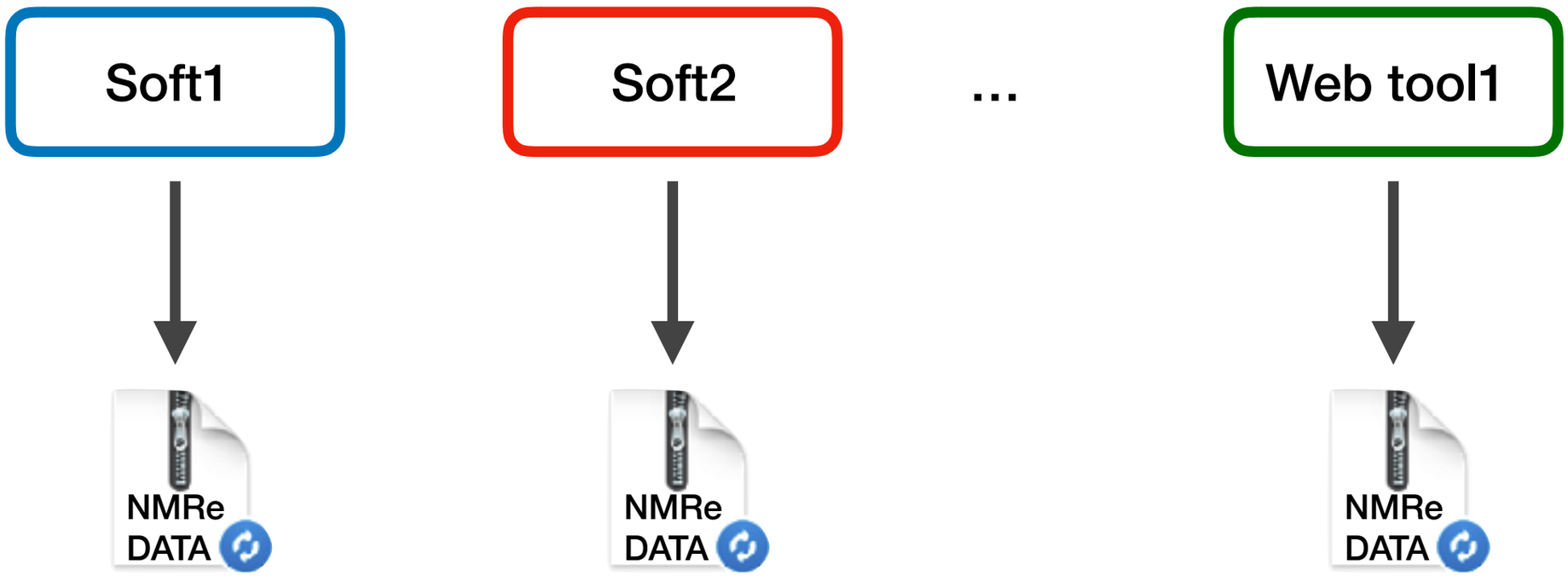
Database + visualisation + assignment tool + …

Compatible software and web service

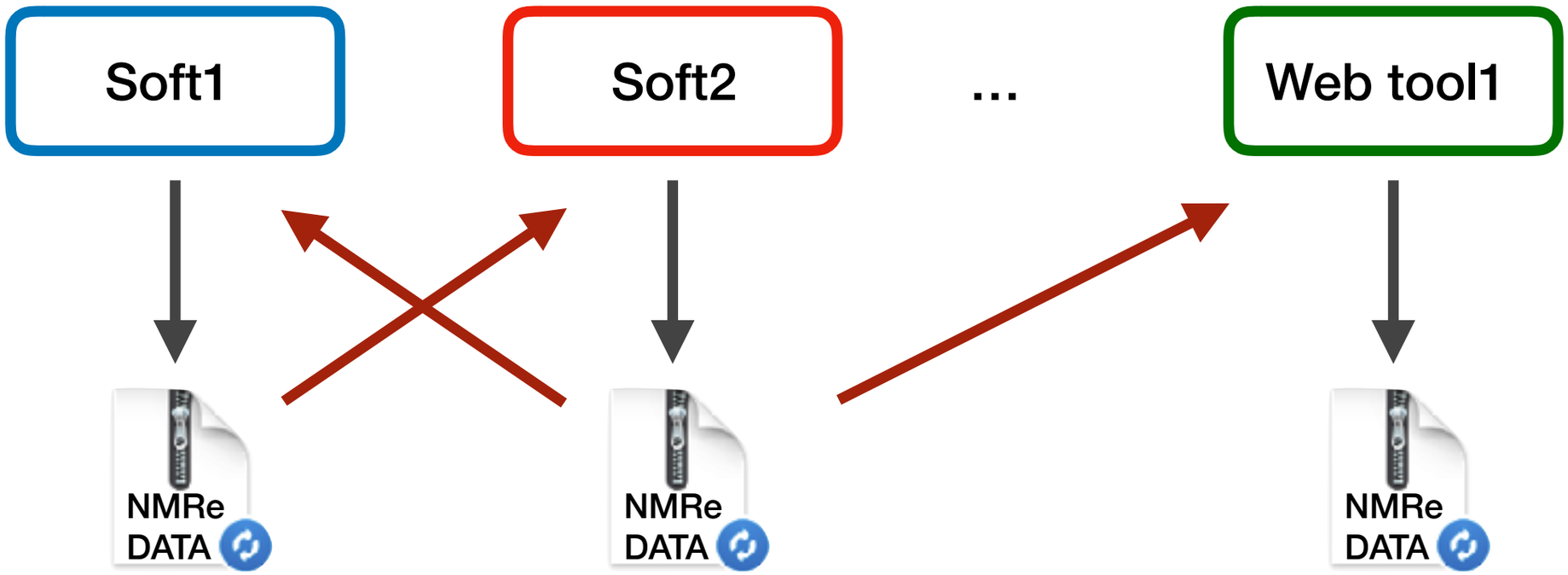
Announced Software & tools

Software Platform	Product/tool	Developer	Operating system	Version	NMReDATA	NMR Record	Examples of output
TopSpin	CMCse	Bruker	Windows, Linux and MAC OS X	V. ?	write	write	
Mnova	Mnova NMR	Mestrelab	Mac OS, Windows, Linux?	Announced for Q1 2018	?		
Matlab/Octave	NMReDATA_View NOMAD	Damien Jeannerat Tomas Lebl	Any system running matalab/octave	V0 (will be on GitHub) when ready for test	read	read	
Firefox/Google Chrome		Julien Wist	Any running Firefox/Google Chrome		generate	generate	

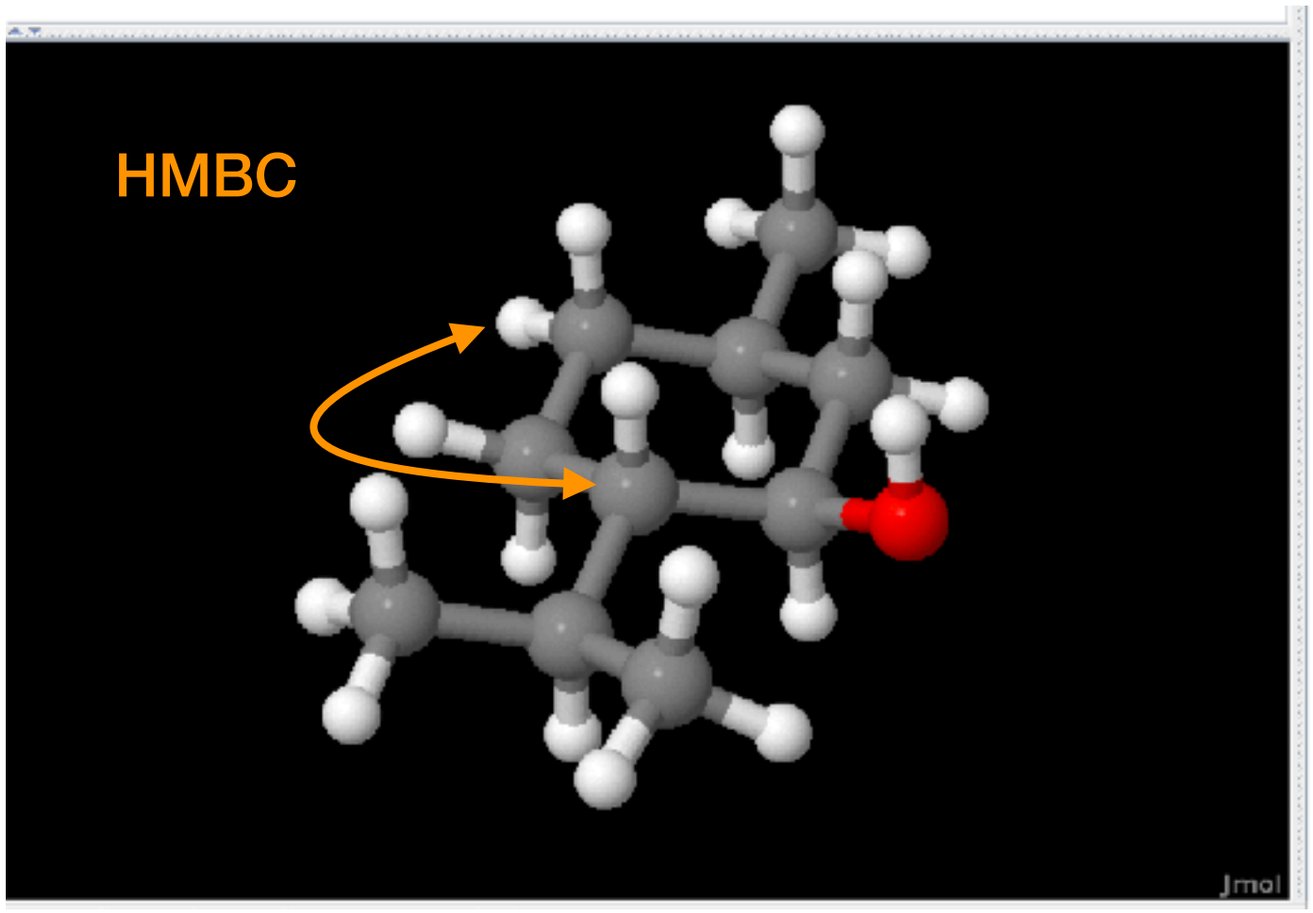
Need certification



Need certification



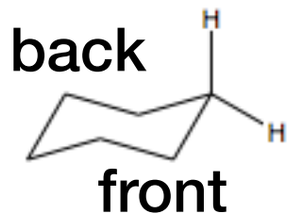
Need Visualizer/Validator



Need tutorial

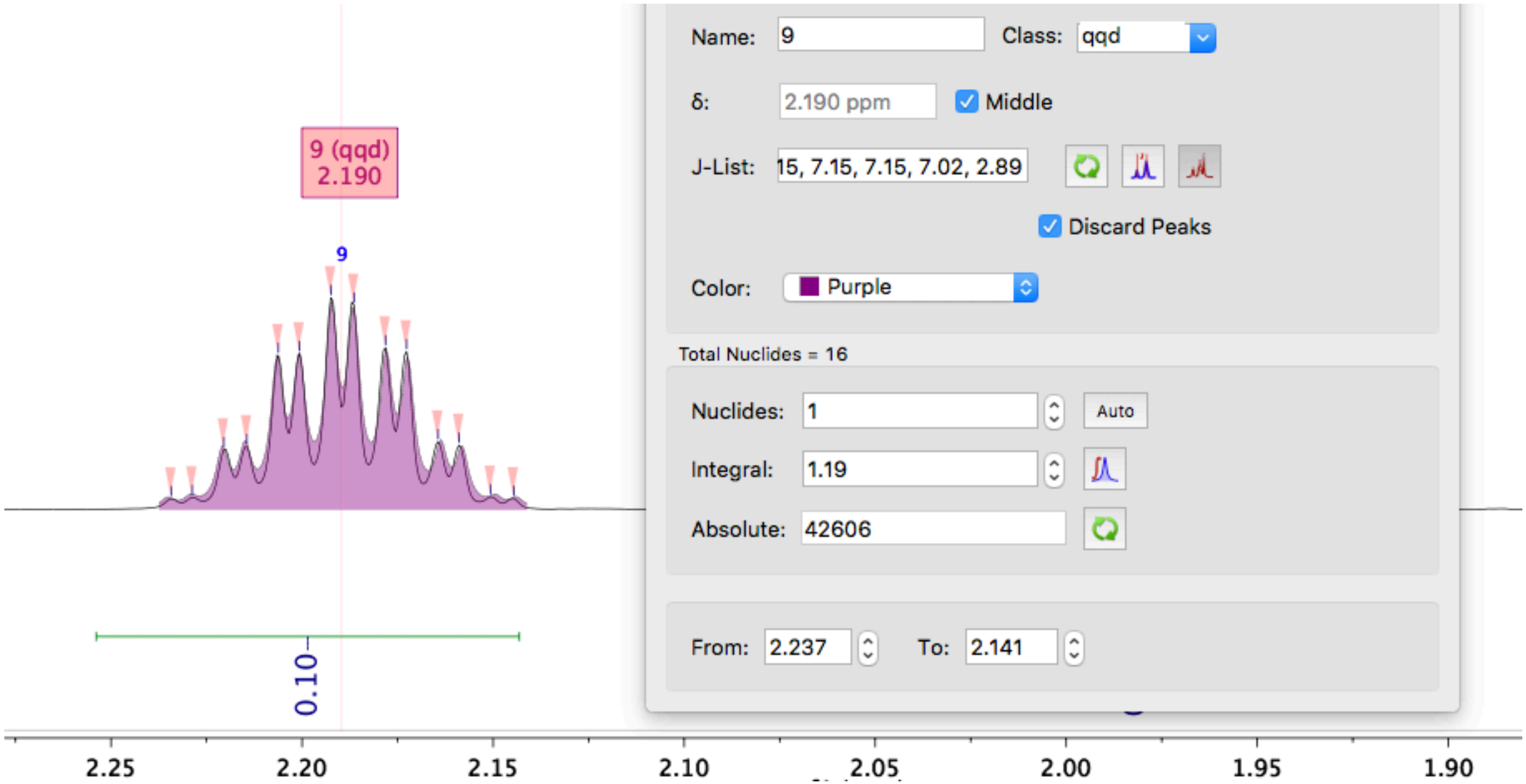
Explicit H when possible/known

Watch for “conventional” explicit information




```
dj-air:3 djeanner$ cat ~/dropbox/demo.mol
demo.mol.sb-4f25a5d6-lDQsBy
  ChemDraw07041811372D

  8  8  0  0  0  0  0  0  0  0999 V2000
   -0.9467   -0.0553    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.3592   -0.7697    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.5659   -0.5430    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.2321   -0.7697    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.6447   -0.0553    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.1486   -0.2819    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.6447    0.7697    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.3592   -0.4678    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
  1  2  1  0
  2  3  1  0
  3  4  1  0
  4  5  1  0
  5  6  1  0
  6  1  1  0
  5  7  1  0
  5  8  1  0
M  END
```

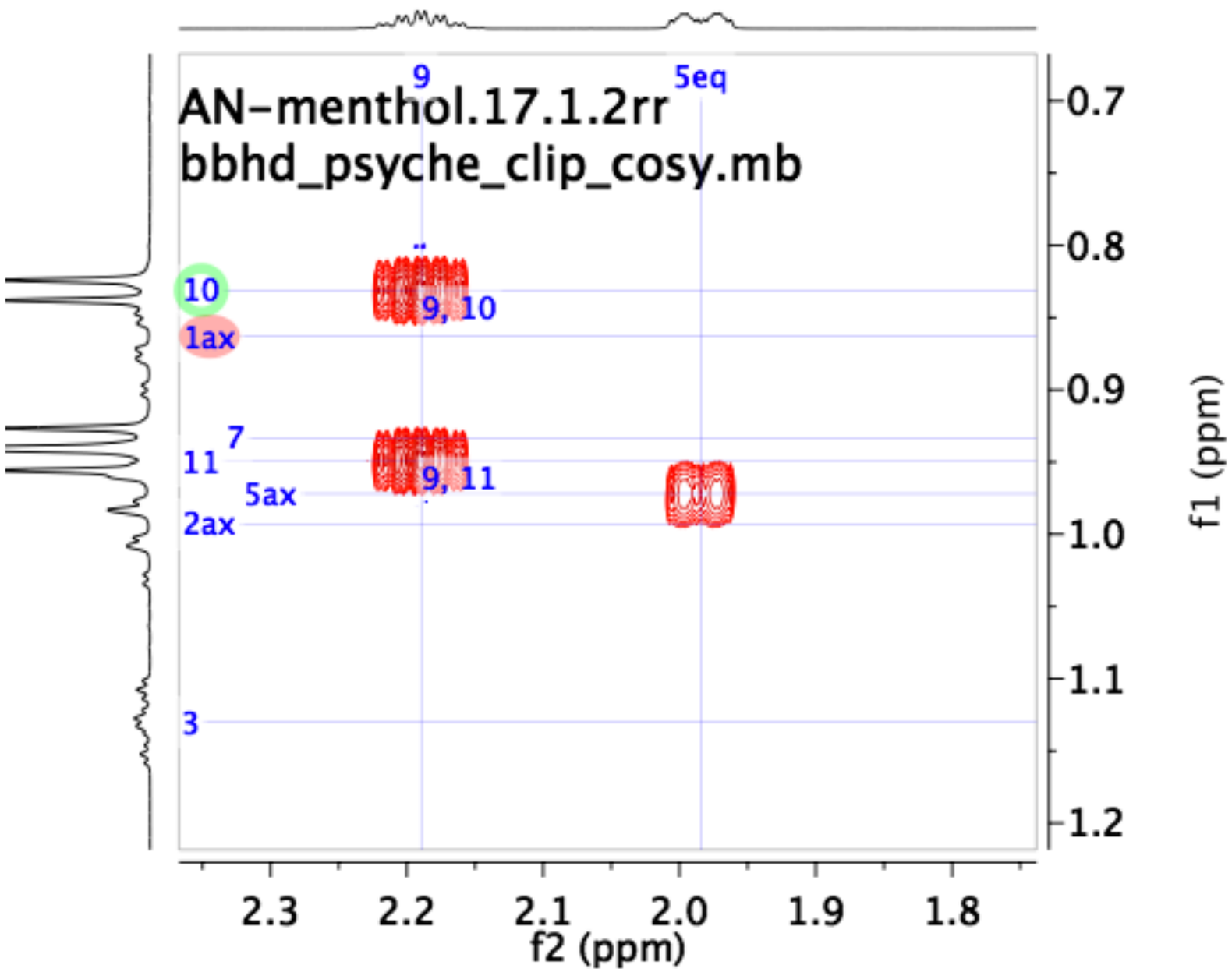
Improve work when exploiting spectra



Improve work when exploiting spectra

Atom	Chemical	Quality	COSY	Predicted	J	NOE	HSQC
1 C	34.57						1b, 1a, 1eq, 1ax
1a...	0.86	-0.31			12.75(...		1
1e...	1.68		☑ 1...		12.75(...		
2 C	23.14						2a, 2eq, 2ax
2a...	0.99		☑ 1...		3.30(1...		2
2e...	1.63		☑ 1...		3.20(1...		2
▼ 3 C	50.16						3
H	1.13		☑ 4		12.76(...		3
▼ 4 C	71.59						4
H	3.43		☑ 1...		9.90(...		4
5 C	45.06						5b, 5a, 5eq, 5ax
5a...	0.97		☑ 4		10.90(...		5
5e...	1.98		☑ 4		4.50(...		5
▼ 6 C	31.62						6
H	1.44		☑ 1...		6.58(...		6
▼ 7 C	22.23						7
	0.93				6.58(6)		7
▼ 9 C	25.84						9
H	2.19		☑ 1...		2.72(3...		9
▼ 10 ...	16.10						10
	0.83		☑ 9		6.98(9)		10
▼ 11 C	20.99						11
	0.95		☑ 9		7.05(9)		11
▼ 12 ...							
H	1.33..1...		☑ 4		4.80(4)		

Improve work when exploiting spectra

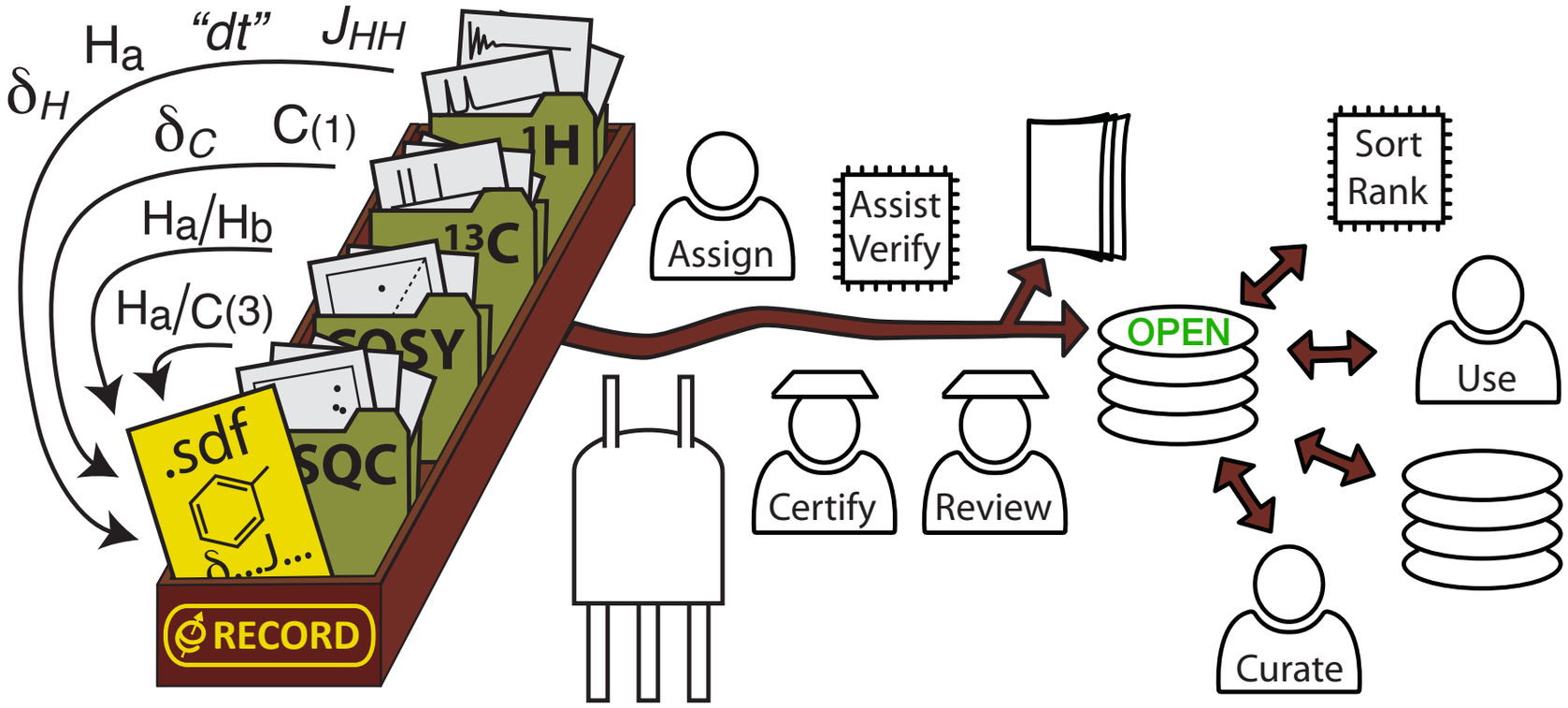


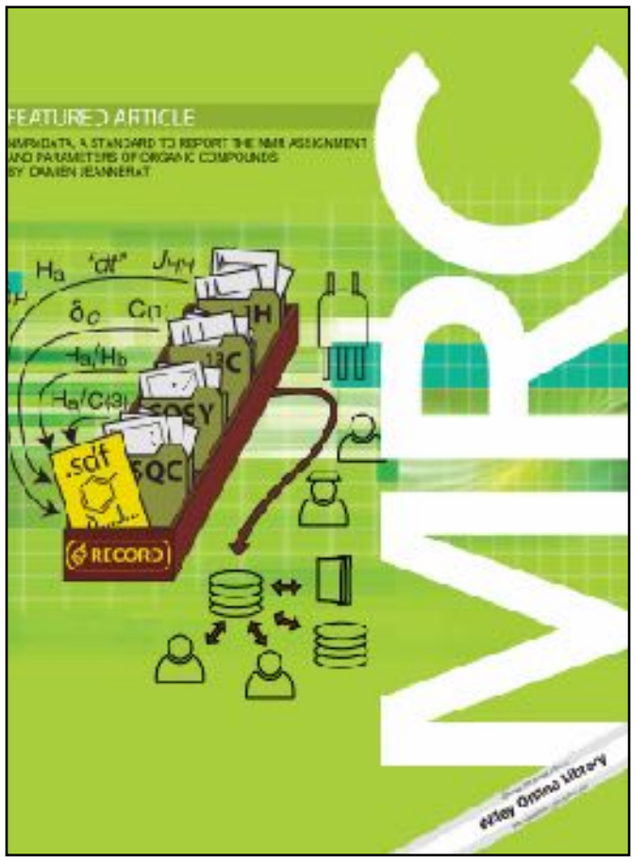
IUPAC, CODATA, FAIRness

Spectra :
Manufacturer's format
Jcamp (simulations, be FAIR)

Conclusion

Mometum
Board of advisers / deciders
Support / Certification (free for non-profit….)





Pupier, M.; Nuzillard, J.-M.; Wist, J.; Schlörer, N. E.; Kuhn, S.; Erdelyi, M.; Steinbeck, C.; Williams, A. J.; Butts, C.; Claridge, T. D. W.; Mikhova, B.; Robien, W.; Dashti, H.; Eghbalnia, H. R.; Farès, C.; Adam, C.; Kessler, P.; Moriaud, F.; Elyashberg, M.; Argyropoulos, D.; Pérez, M.; Giraudeau, P.; Gil, R. R.; Trevorrow, P.; Jeannerat, D., NMReDATA, a standard to report the NMR assignment and parameters of organic compounds. *Magn. Reson. in Chem.* **2018**.

The NMReDATA Initiative

nmredata.org

Academic partners:

Julien Wist[1,§], Jean-Marc Nuzillard[2], Nils E. Schloerer[3], Stefan Kuhn[3], Marion Pupier[4], Mate Erdelyi[5], Christoph Steinbeck[6], Antony J. Williams[9,&], Craig Butts[10], Bozhana Mikhova[11,*], Damien Jeannerat[4,§]

Industrial partners:

Wolfgang Robien

Kessler Pavel[#], Fabrice Moriaud,[#] Mikhail Elyashberg[%], Dimitris Argyropoulos[%], Manuel Pérez[&,§]

Publishing partner:

Patrick Giraudeau[7,§], Roberto R. Gil[8,@], Gary Martin[‡,@], Paul Trevorrow[£]

[1] **University of Valle**, Cali, Colombia
[2] CNRS and **University of Reims-Champagne-Ardenne**, Reims, France
[3] IDNMR, **University of Cologne**, Cologne, Germany
[4] Department of organic chemistry, **University of Geneva**, Geneva, Switzerland
[5] Department of Chemistry - BMC, **University of Uppsala**, Sweden
[6] Cheminformatics and Chemometrics, **Friedrich-Schiller-University Jena**, Germany
[7] CEISAM, **University of Nantes**, Nantes, France
[8] Department of Chemistry, **Carnegie Mellon University**, Pittsburgh, USA
[9] National Center for Computational Toxicology, **EPA**, USA
[10] **University of Bristol**, UK
[11] Institute of organic chemistry, **Bulgarian academy of sciences**, Bulgaria

[#] **Bruker BioSpin GmbH**, Rheinstetten, Germany
[%] **ACD/Labs**, Toronto, Canada
[&] **Mestrelab Research**, Santiago de Compostela, Spain
[‡] **Merck and co**. New-Jersey, USA

Magnetic Resonance in Chemistry, Wiley, Chichester, UK
[@] Coeditors in Chief
[*] Member of the *Editorial board*
[§] Member of the *Associate board*
[&] Member of the *Advisory board*
[£] Executive journal editor

Follow the progress of the initiative on

www.nmredata.org

POSTER 376