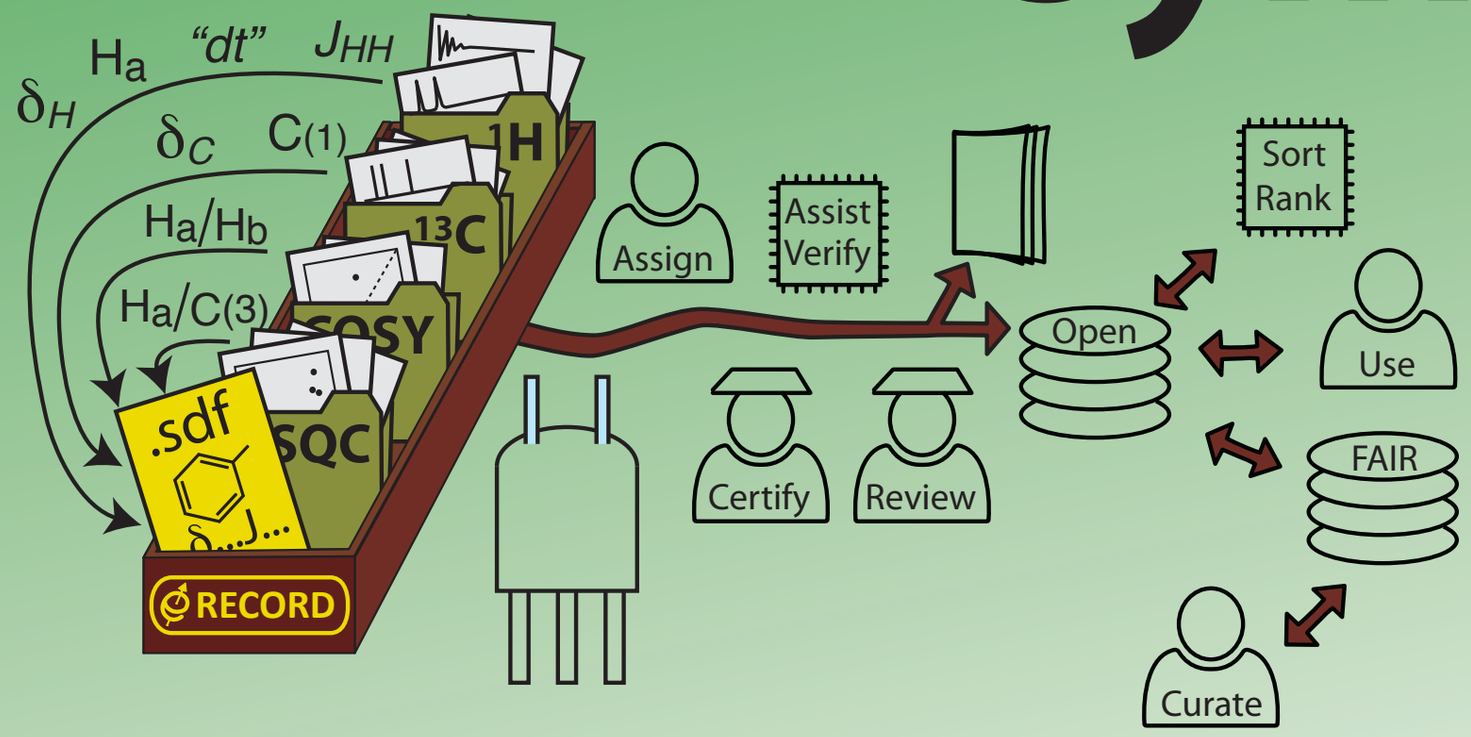
1st NMReDATA symposium



Thursday
26 Sept. 2019

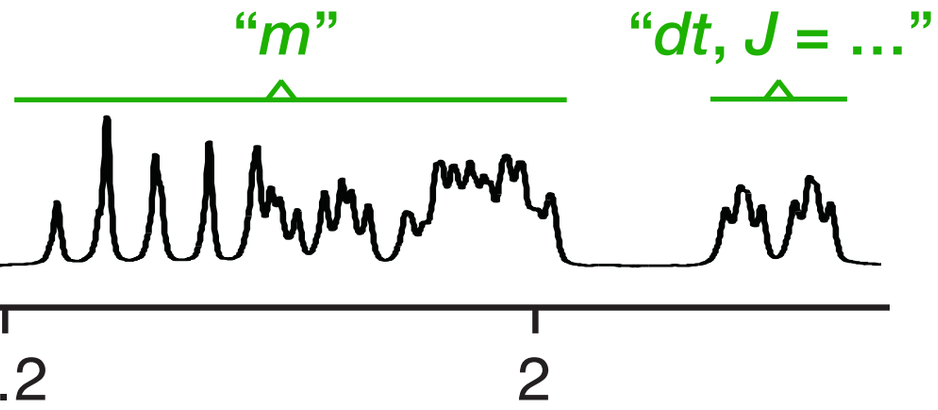
Porto, Portugal

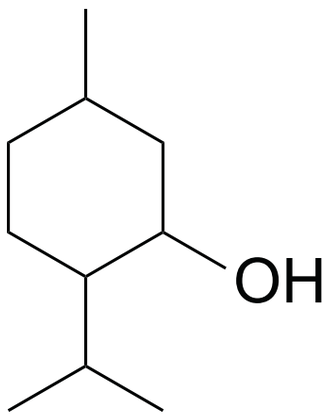
www.nmredata.org

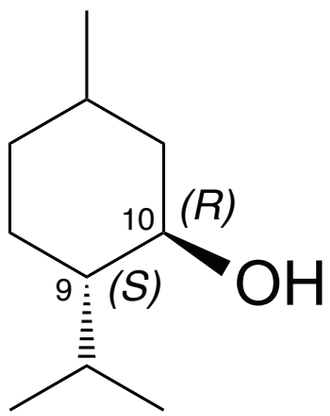
Welcome!

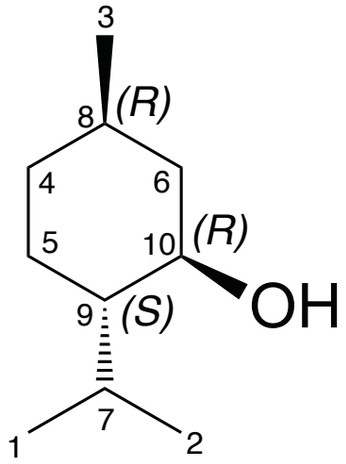
The NMReDATA initiative

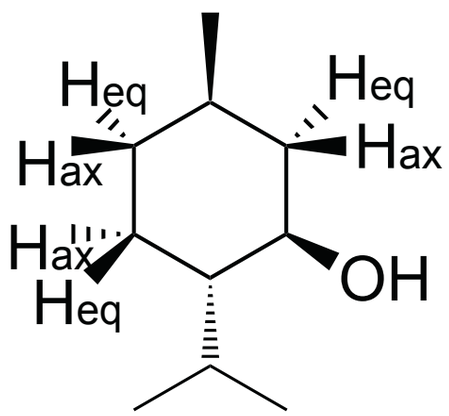
The NMReDATA initiative

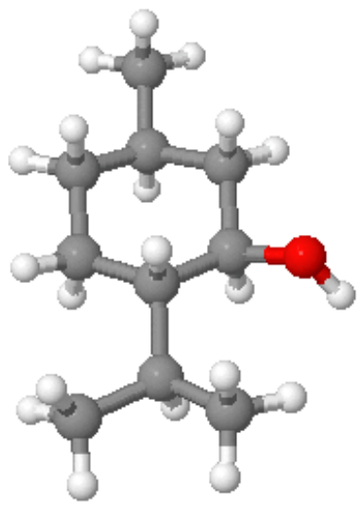






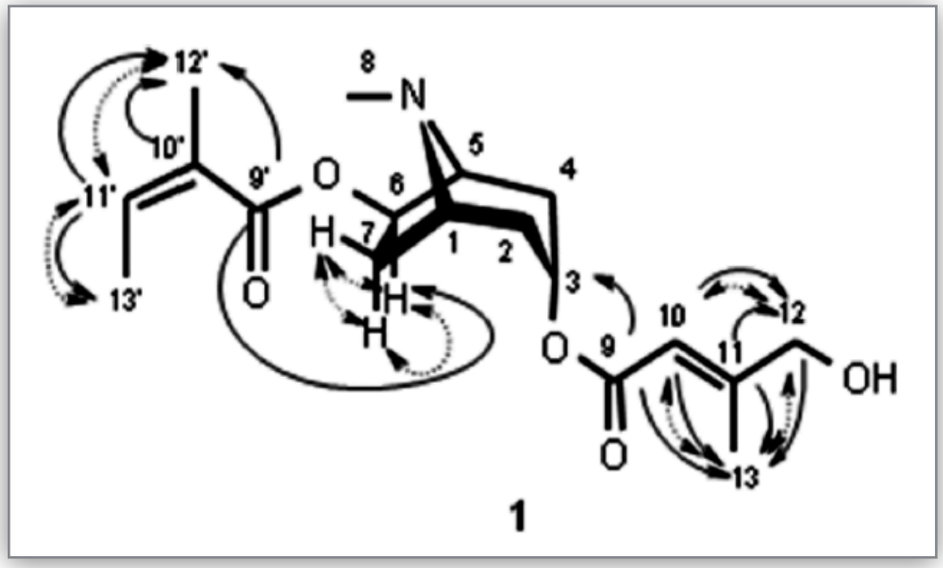




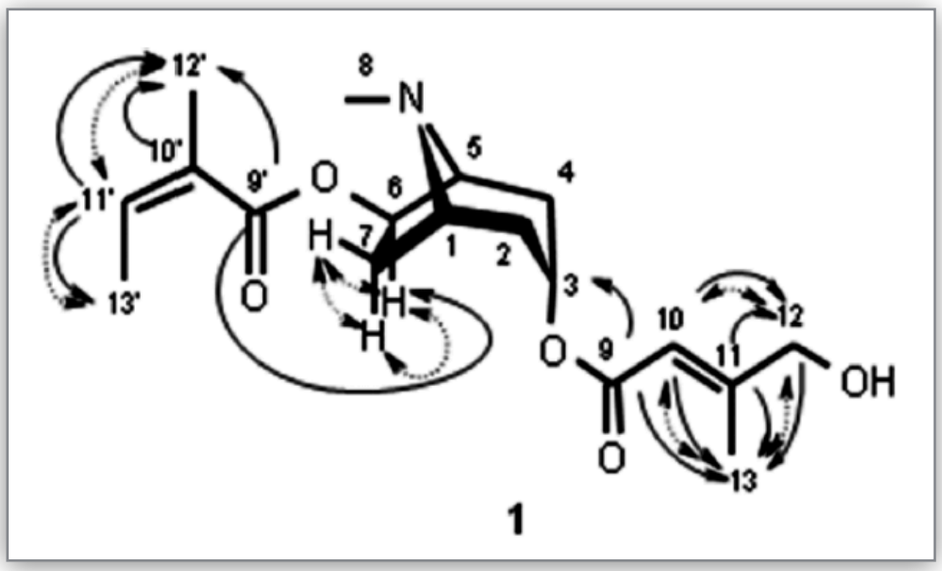


The NMReDATA initiative

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 (15), 95 (76), 94 (100), 83 (14), 82 (13); CIMS *m/z* 256 (62), 238 (14), 222 (91), 140 (48), 122 (100); HREIMS *m/z* 338.1973 ($C_{18}H_{28}NO_5$ $[M + H]^+$, requires 338.1967).



The NMReDATA initiative



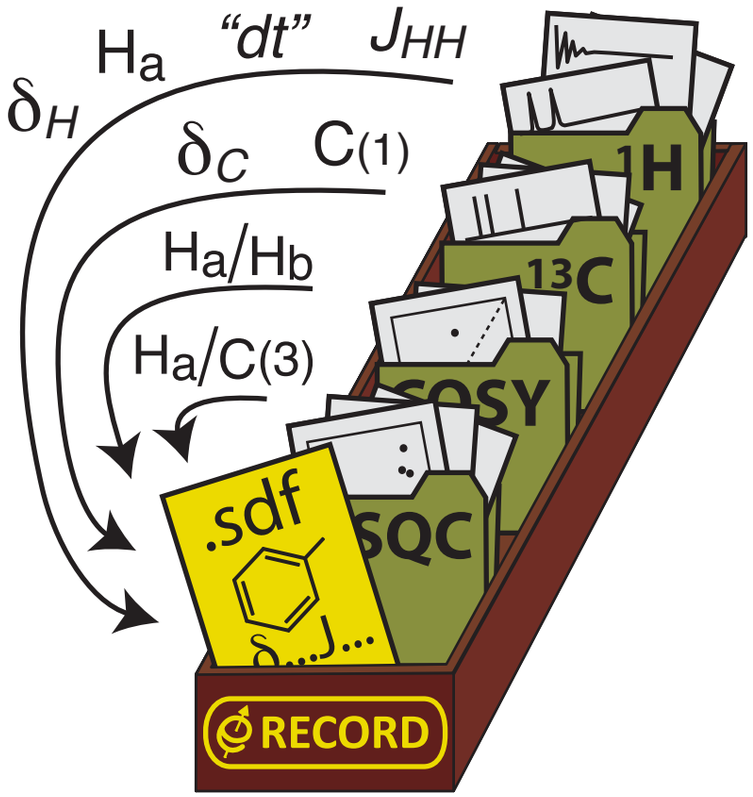
1

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_{endo}	2.38 br s	31.9	2.43 br s		2.39−2.43 br s
	CH_{exo}	2.14 s		2.22 s		2.14 s
5	66.9 CH	3.63 s	67.4	3.79 s	66.0[c]	3.90 s
6	76.5 CH	5.64 s	74.8	5.62 s	78.0[a]	5.64 s
7	34.2 CH_{endo}	2.83 br s	34.3	2.88 s		2.95 s
	CH_{exo}	2.38 br s		2.36 br s		2.41−2.43 br s
8	39.0 CH_3N	2.77 s	38.5	2.88 s	38.5[a]	2.95 s
9	165.5[b] qC		165.5[b]			
10	112.4 CH	6.05 s	112.3	6.05 s	119.5[c]	6.55 s
11	160.5[c] qC		160.7[c]		154.0[c]	
12	65.9 CH_2	4.10 s	65.8	4.11 s	174.0[c]	
	OH	3.33 s		3.36 s		
13	14.6 CH_3	2.11 s	14.7	2.11 s	14.6[a]	2.31 s
9′	167.4[c] qC		166.3[b]		178.5[c]	
10′	127.3[c] qC/CH		114.8	5.74 s	115.5[c]	5.75 s
11′	139.0 CH/qC	6.19 s	159.3[c]		157.0[a,c]	
12′	19.4 CH_3	1.91 s	19.3	2.19 s	19.0[c]	2.19 s
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 (isomer subfraction). [c] Based on HMBC.

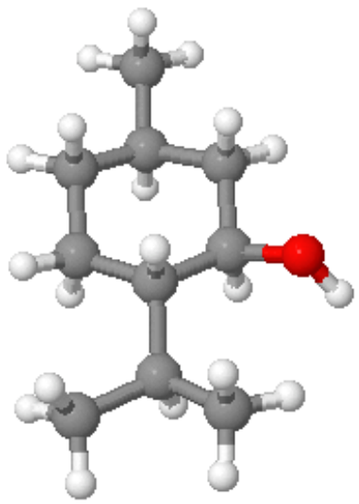
The NMReDATA initiative



.sdf

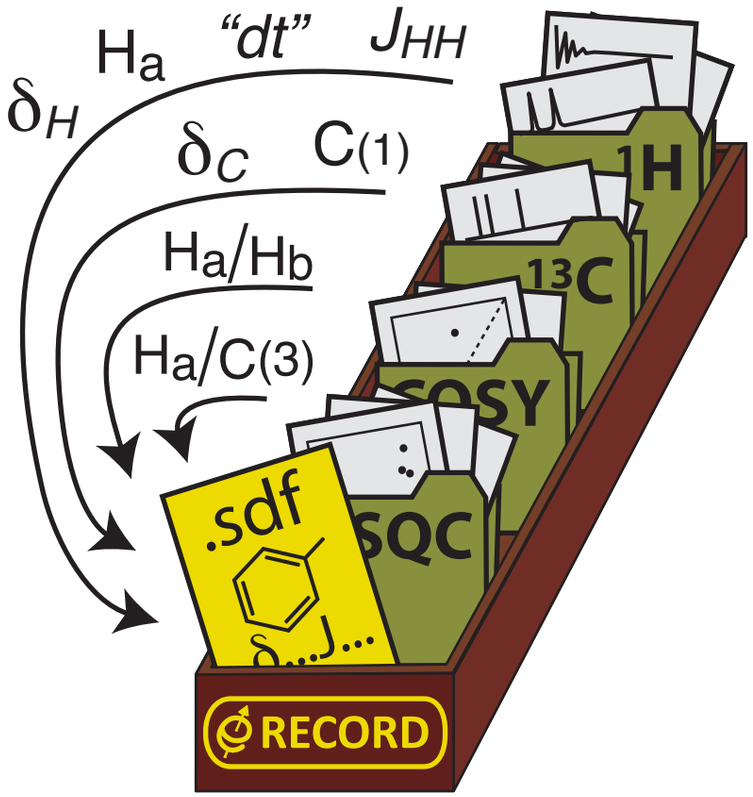
≡

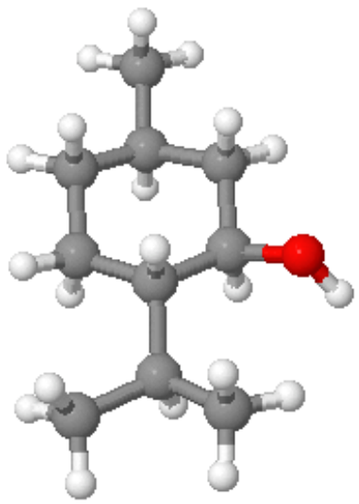
.mol + <metadata>



```
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\
```

The NMReDATA initiative

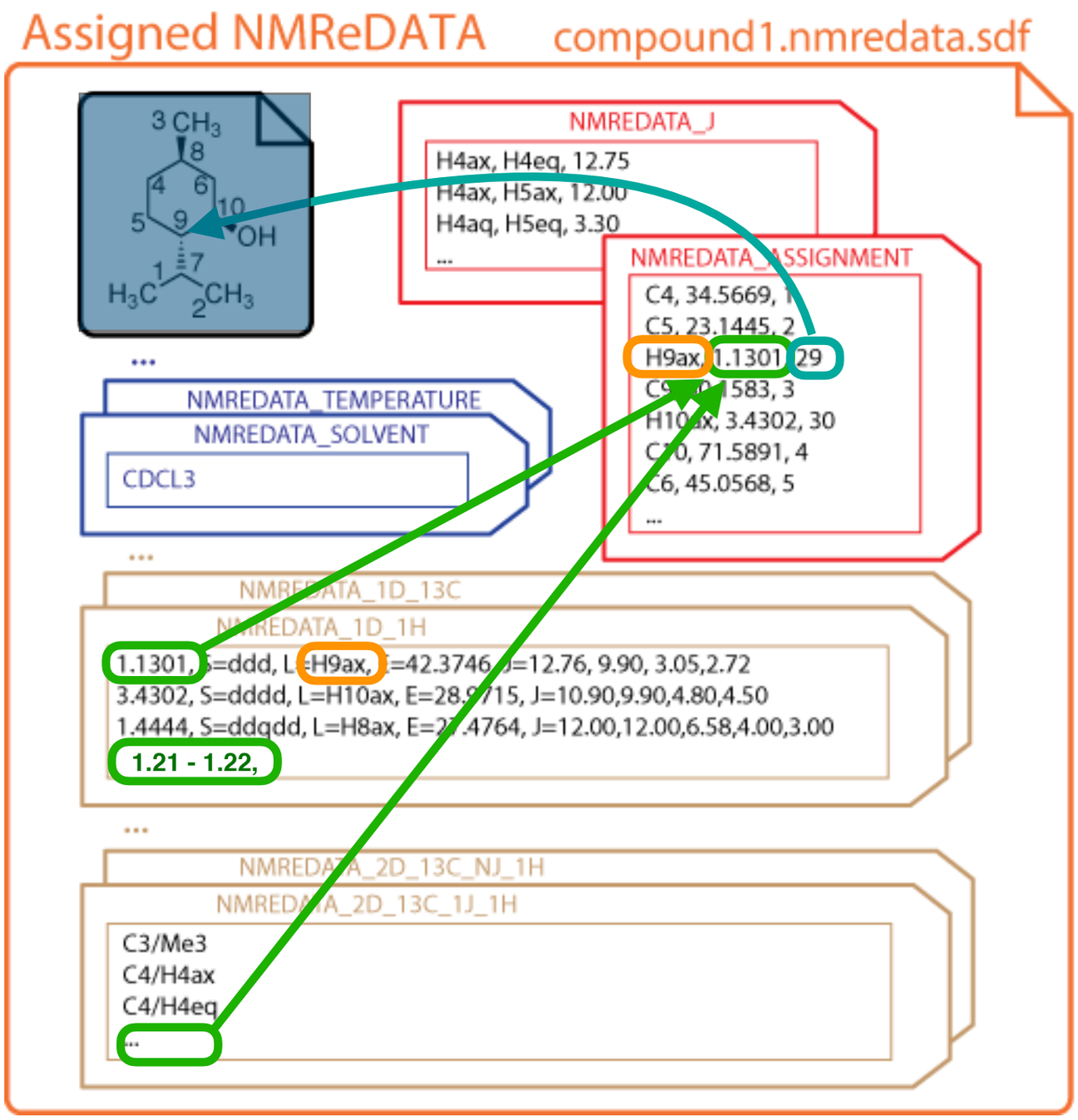




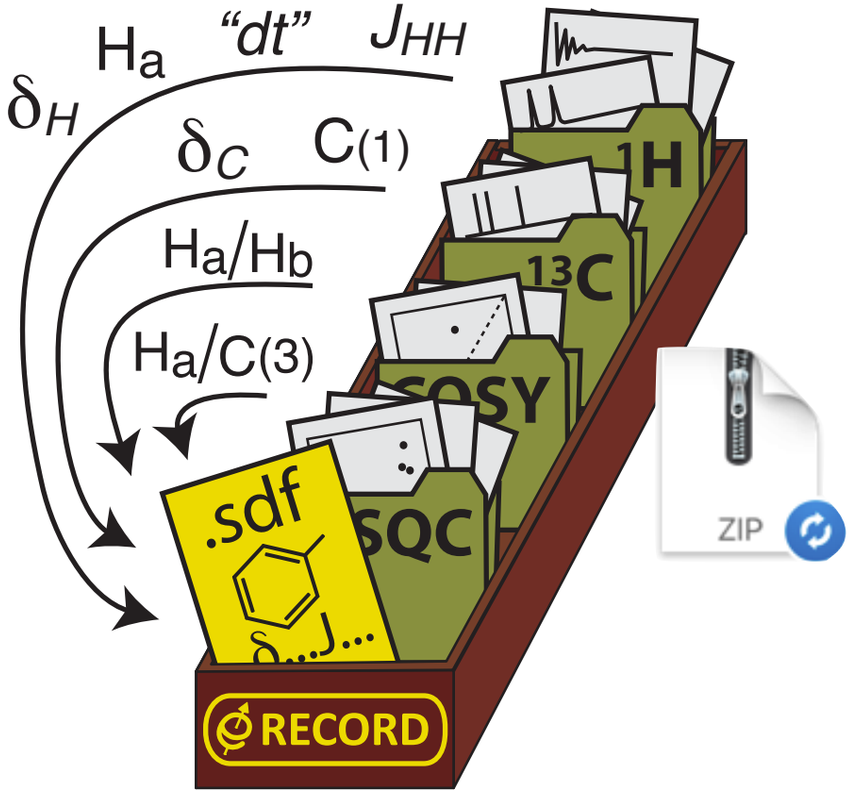
.sdf

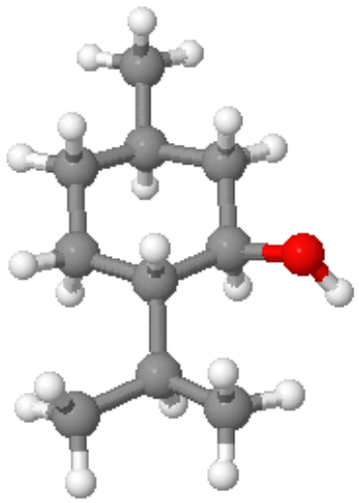
≡

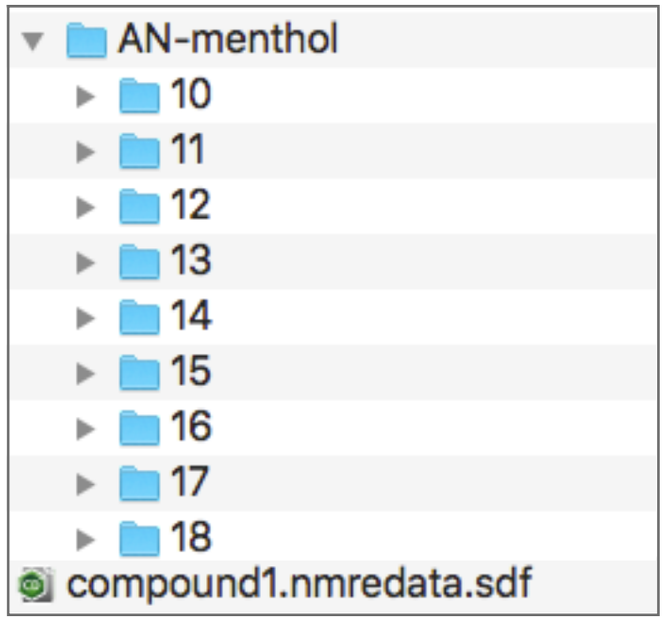
.mol + <metadata>



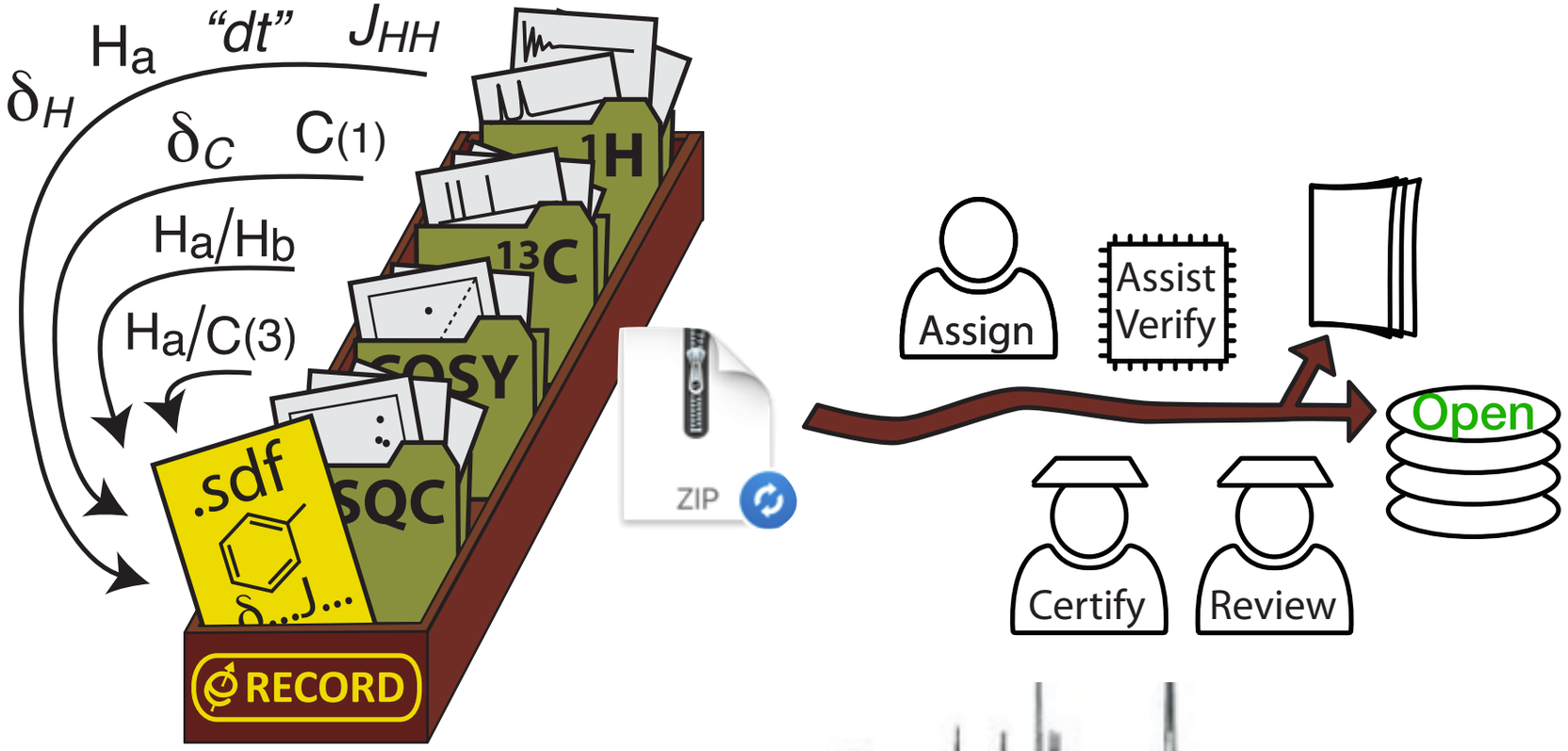
The NMReDATA initiative

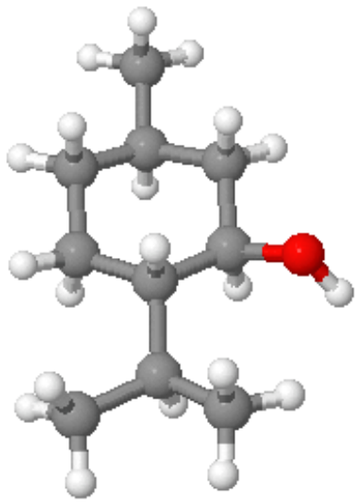


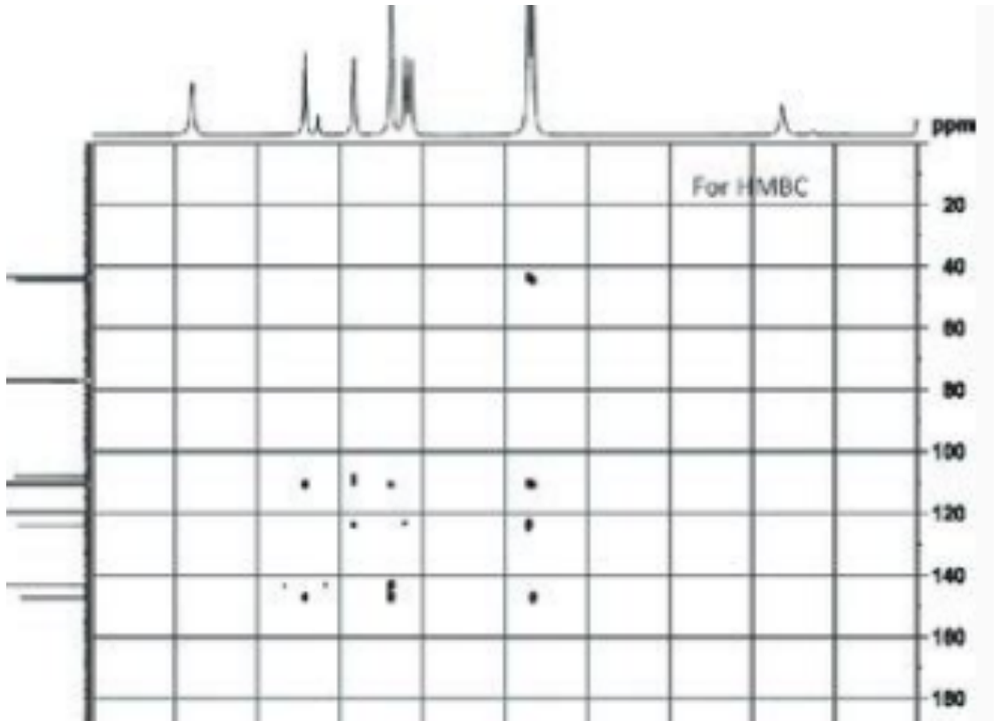




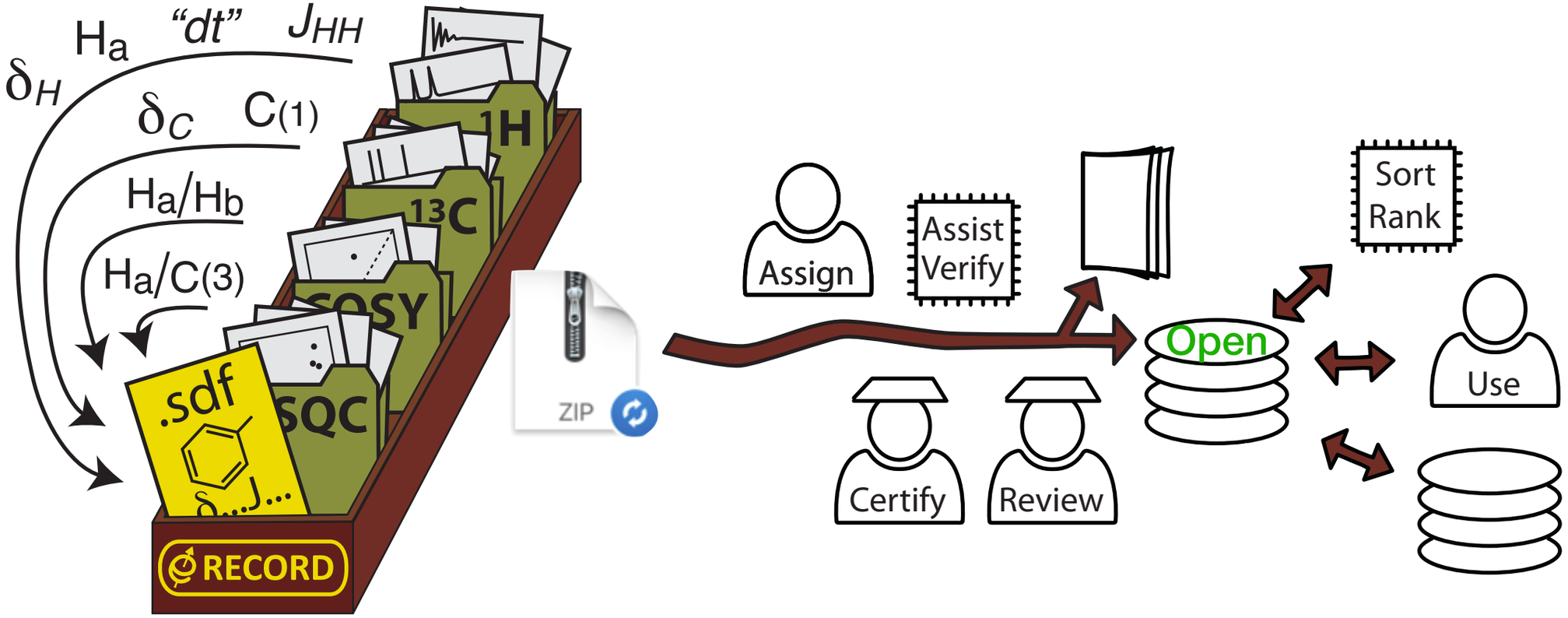
The NMReDATA initiative

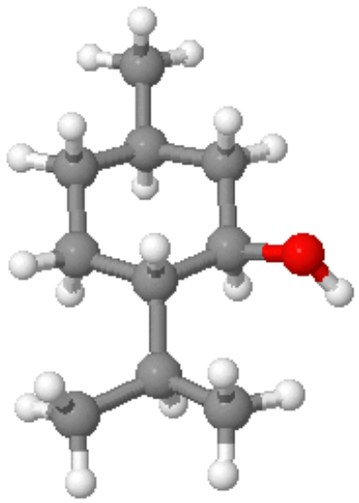






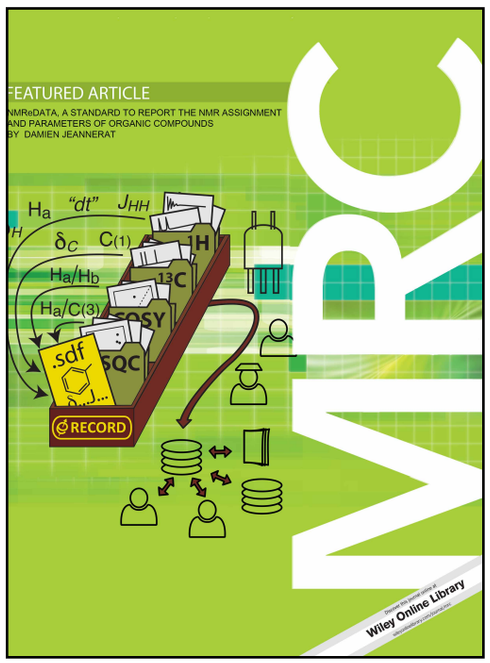
The NMReDATA initiative





Findable (J, δ, *etc.)*
Accessible (from open database*)*
Interoperable (SDF is a standard)
Reusable (J, δ, spectra, structures, fragments, *etc.*)

The NMReDATA initiative



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

Program

Relevance of the NMReDATA Initiative in chemistry

9:00-9:15 Forwords on the NMReDATA Initiative, Damien Jeannerat

9:15-10:00 Feature presentation

Jonathan Bisson, University of Illinois Chicago, USA

What can we do with RAW NMR data and spin parameters

10:00-10:40 Short talks

Wolfgang Robien, University of Vienna, Austria

A few remarks on wrong structures in the literature

Nils Schloerer, University of Cologne, Germany

Teaching NMR data handling, electronic assignment and CASE at the university

10:40-11:00 Coffee Break

Available software and tools relevant to the NMReDATA Initiative

11:00-12:40 Short talks

Stefan Kuhn, De Montfort University, Leicester, UK

NMReDATA software and nmrshiftdb2

Pavel Kessler, Bruker Biospin, Germany

Bruker implementation of NMReData

Mitcheell Maestre-Martinez, Mestrelab, Spain

Mnova meets NMReData: automation workflows and new opportunities

Dimitris Argyropoulos, ACD/Labs, Canada

Implementing the NMREDATA format into your workflows using

Sina Kazemi, SIGNALS, Germany

LOGS - a natural fit for NMReData

12:40-13:30 Lunch Break

The NMReDATA initiative

Further development of NMReDATA

13:30-15:10 Short talks

Robert Hanson, St. Olaf College, Northfield, MN, USA
Putting it all together: Fully automated NMR spectrometer, web-based analysis, and spectral simulation with 2D/3D structure correlation for first-year organic chemistry

Angel Herráez, University of Alcalá, Spain
NMReDATA J_reader: an HTML interface for displaying the contents of NMReDATA files, molecular structure, NMR data and spectra

Jean-Marc Nuzillard, University of Champagne Ardenne, France
NMReDATA file validation through Computer-Assisted Structure Elucidation

Damien Jeannerat, NMReDATA Initiative, Switzerland
Validation of NMReDATA by spectral simulation

Tomas Lebl, St Andrews University, UK
NOMAD - NMR Online Management and Datastore

15:10 - 15:40 Coffee break

Round table discussion

15:40 - 16:20

Discussion of open issues with the format

Structure, funding and organisation of the NMReDATA Initiative

16:20 - 16:30

Closing remarks