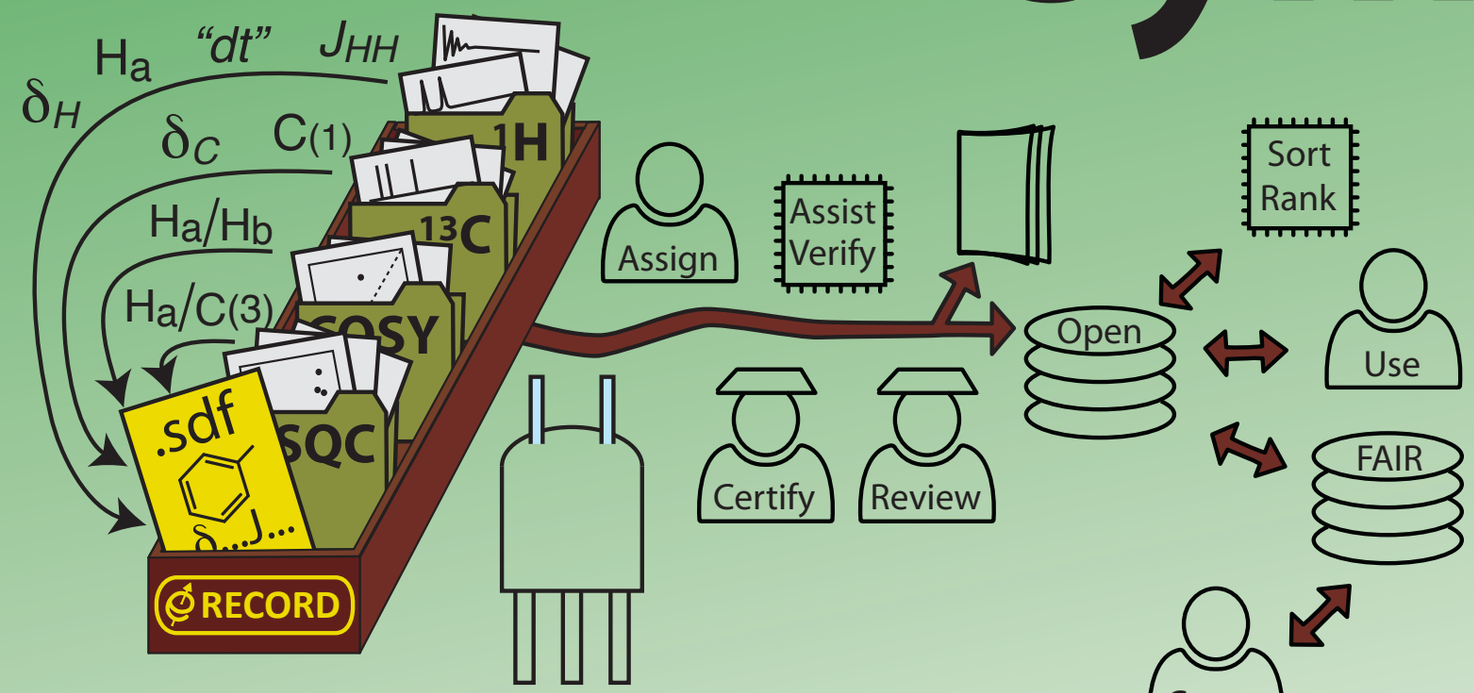
1st NMReDATA symposium



Thursday
26 Sept. 2019

Porto, Portugal

www.nmredata.org

Discussion

http://www3.uah.es/mol_play/NMReDATA/reader46.htm

Angel Herraez (*JSmol*, Bob Hanson)

File contents

(click on items to display them if feasible)

menthol_1D_1H_assigned_J.zip
- AN-menthol
  - compound1_special_labels.n...
  - compound1_with_jcamp.nm...
  - compound1.nmredata.sdf
- jcamp_nmr_spectra
  - only_one_HH_coupling_in_J...
  - wild_JCH_coupling.sdf
  - with_char_10.sdf

NMReDATA tags

(click on each header to unfold/fold its contents)

VERSION
LEVEL
ID
SOLVENT
ASSIGNMENT
J
1D_1H

model number 2:

2~VERSION
2~ASSIGNMENT
2~J
+

Other tags

+

Item contents

SDF header

model number 1:

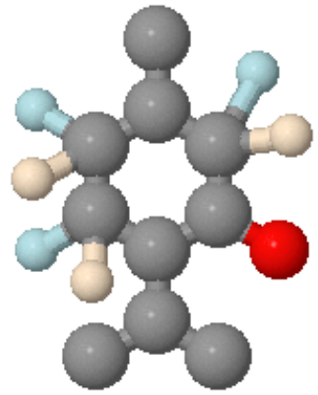
ChemDraw10231713492D

model number 2:

3D model
__Jmol-14_07051907113D 1 1.00000 0.00000 0
3D coordinates generated by JSmol v. 14.29.46

Molecular structure display

compound1.nmredata.sdf



JSmol

assignments
Display: all
Color code: (off)
move labels

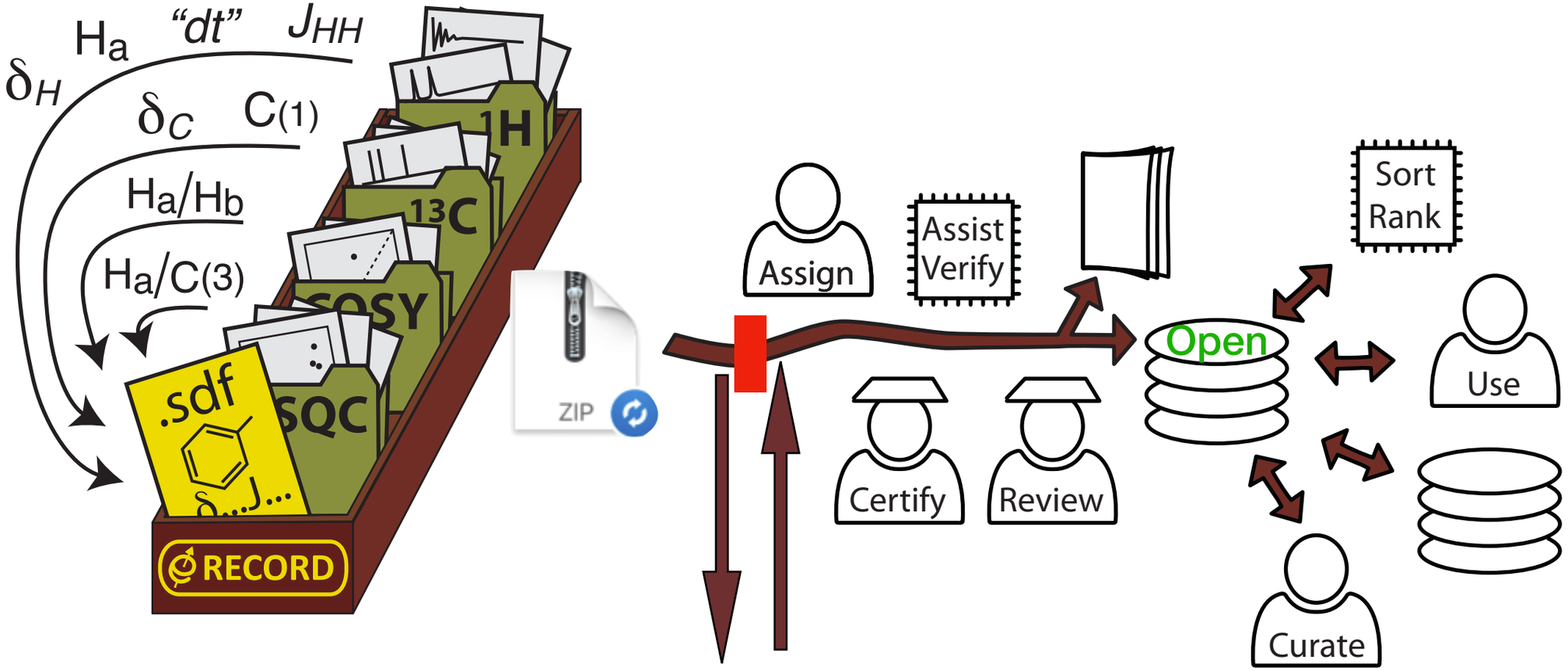
couplings
Display: all
from: J tag
explicit implicit H
J values

add H's & make 3D

expand

bond up
bond down

The NMReDATA initiative



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Make FAIR

.cdx → .mol

Bruker, Varian, Mnova → .jcp

Future development 1

Findable (J, δ, *etc.)*

Accessible (from open database*)*

Interoperable (SDF is a standard)

Reusable (J, δ, spectra, structures, fragments, *etc.*)

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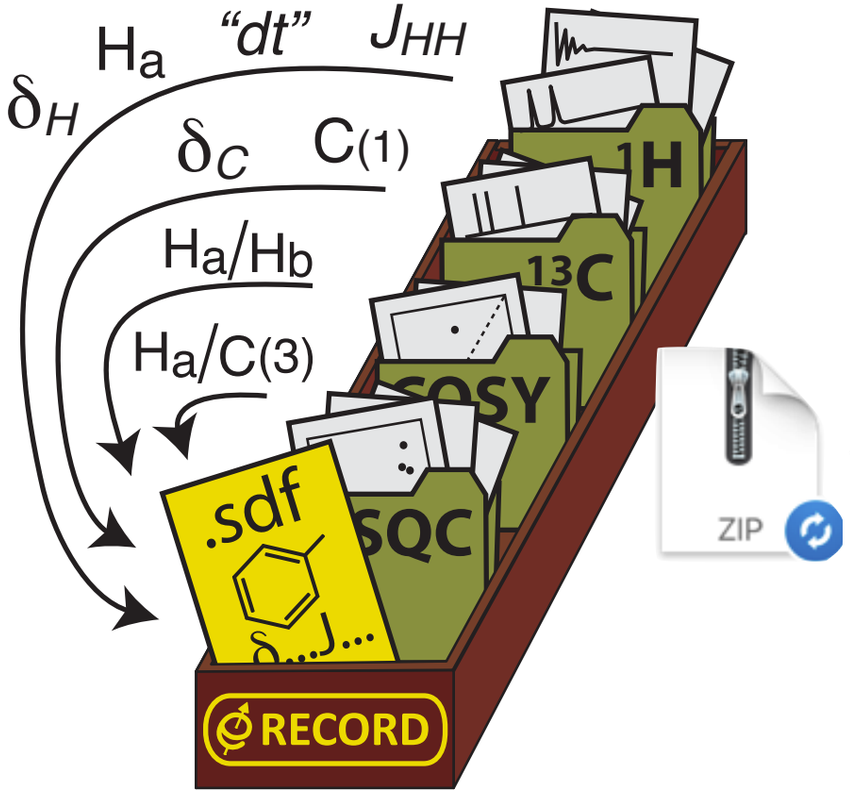

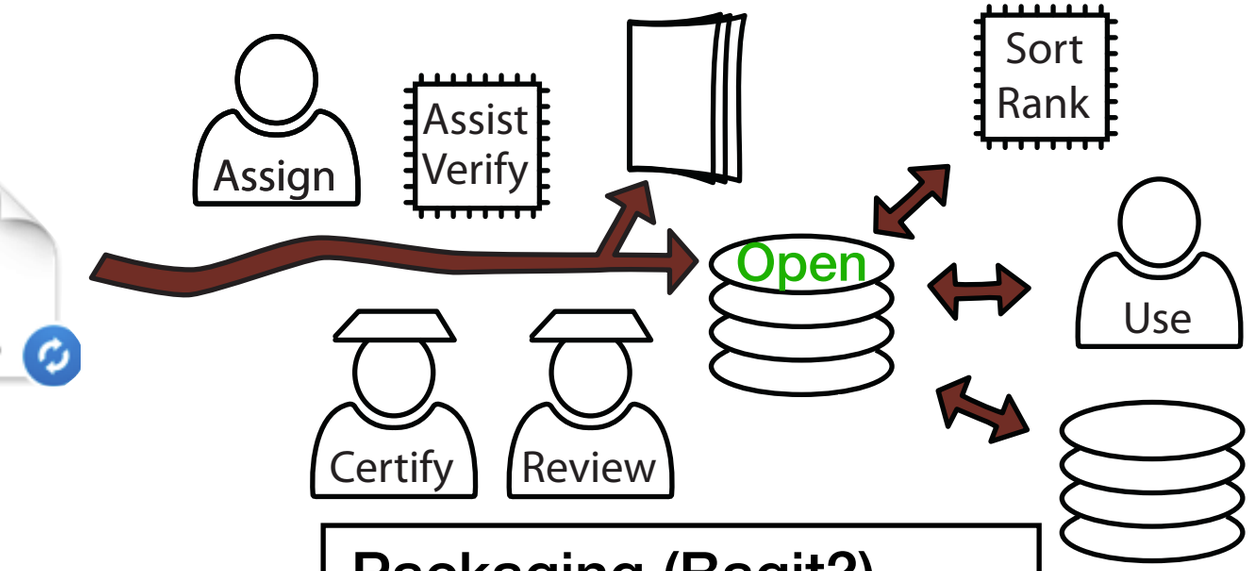

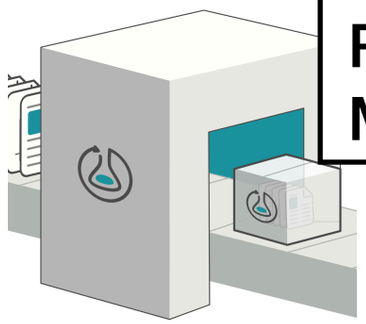

Packaging (Bagit?)
Research object?
Meta data, Schema, *etc.*

Future development 2

NMR DATA

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International Union of Pure and Applied Chemistry

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TEL: +1-919-485-8700 FAX: +1-919-485-8706 EMAIL: secretariat@iupac.org

PROJECT SUBMISSION FORM

for administrative use only	*Submitted* _____ ; # _____
Date	July 20 2019
Project Title	~~Incorporating~~ Development of a standard for FAIR Metadata into Spectroscopic Data Files
Series Title *(if applicable)*	
Task Group Chair	(co-chair) Damien Jeannerat, University of Geneva, NMReDATA Initiative, Switzerland, damien.jeannerat@protonmail.com (co-chair) Robert Hanson, St Olaf College, USA,

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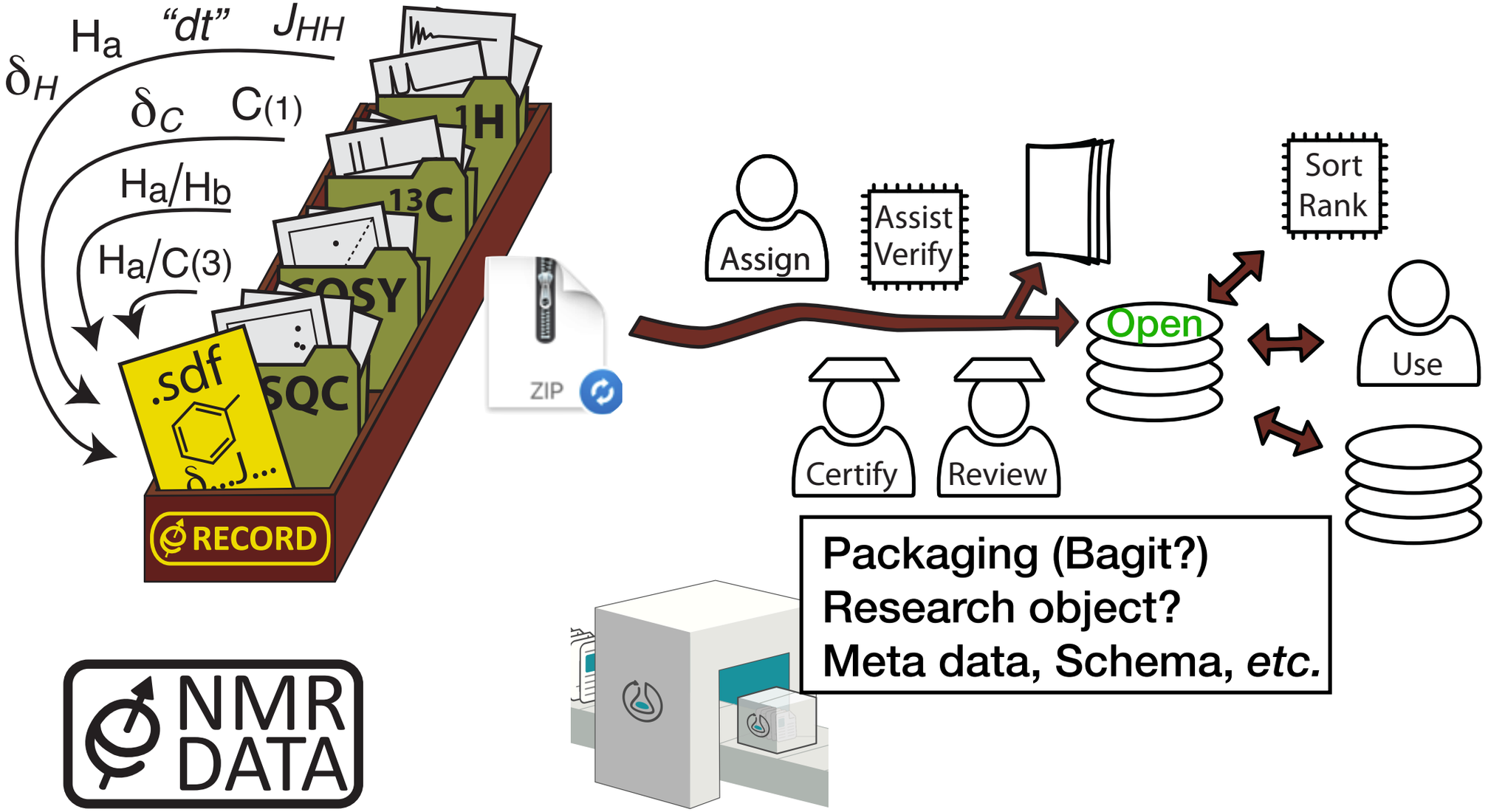

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chemedata.org

Future development 3

Other spectroscopies (UV-Vis, IR, MS, *etc.*)
logfiles (DFT calculations, Modeling, *etc.*)
…

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Versioning (short term)
Github
Chemspider

?

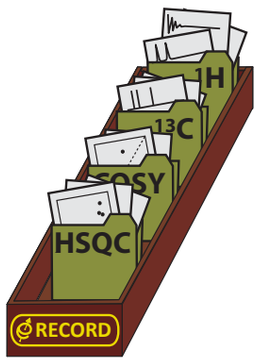
Corrections
additions

Check consistency data/spectra
Logic for Structure Determination

C-search
NMRShiftDB2

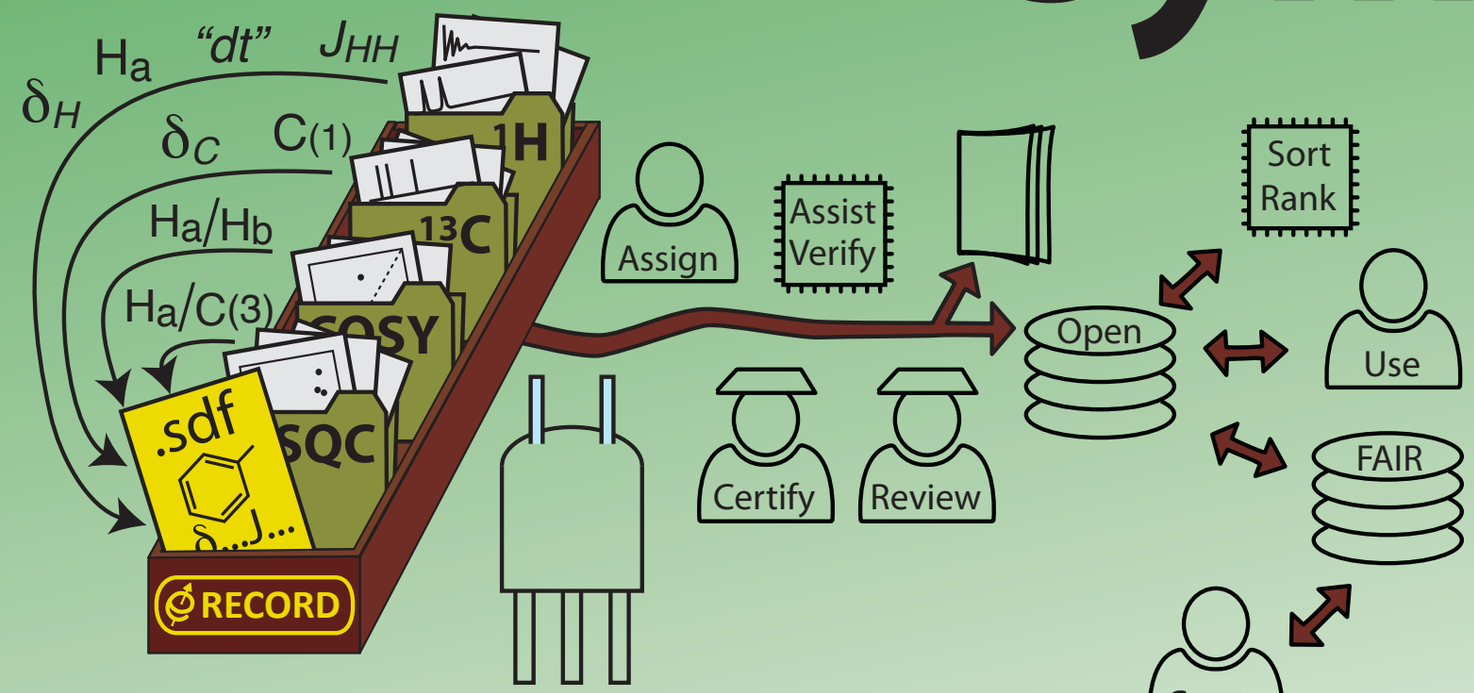
Passed review process
Certified by webtool…

t



Long-term open access
Zenodo, …
University repository, Funding agencie, …

1st NMReDATA symposium



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Discussion

The NMReDATA initiative

SMASH

Craig Butts

…

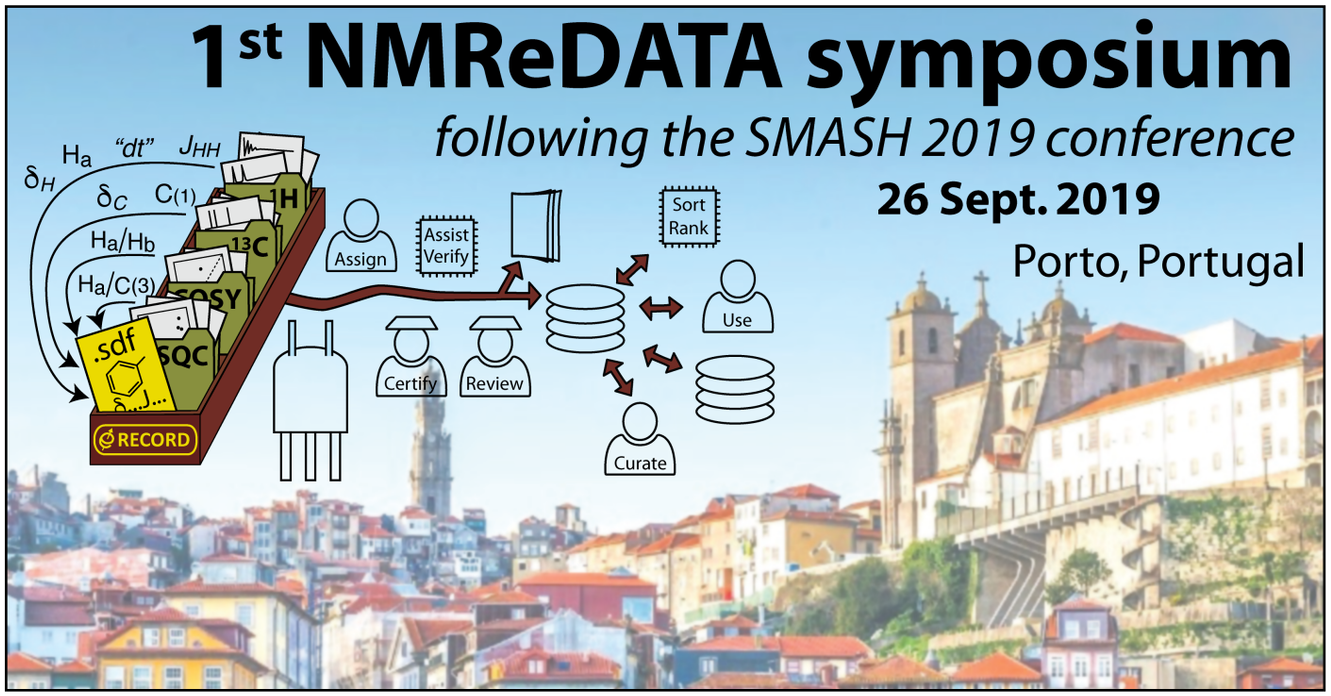
Carla Marchioro

Symposium

Speakers

Paul Trevorrow (Wiley)

co-chair Stefan Kuhn



Keep in touch ….