

# Bruker NMReData Implementation

NMReData Meeting, Porto 2019



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# Outline



- NMReData and NMR Records export
- NMReData import
- Availability
- Technical comments



# NMReData Export



## CMC-se

- Structure elucidation
- Structure validation

Screenshot of the NMReData software interface showing the export process for a CMC-se project (A2).

The main window shows a 2D NMR correlation matrix for a <sup>13</sup>COSY experiment. The x and y axes are labeled with carbon atoms (H1-H14) and their corresponding chemical shifts (e.g., H1 at 10.55 ppm). Correlations are indicated by colored arrows (blue for <, red for >, green for S+, yellow for M, purple for v, cyan for A).

A secondary window titled "NMR Records Export" displays the destination folder as "C:\Users\pavel.kessler".

A third window titled "NMR Records" shows a message: "CMC-se project was exported to C:\Users\pavel.kessler\A2.nmredata.zip".

The right side of the interface features a "Chemical Structures" panel showing a complex organic molecule with numbered atoms (1 through 20) and a list of 152 structures.

# NMReData Export



Screenshot illustrating the NMReData Export process, showing the export of NMR data from a Bruker instrument and its subsequent analysis.

The left window shows a file explorer interface for "Compressed Folder Tools A2". The path is: This PC > SYSTEM (C:) > Users > pavel.kessler > A2.nmredata.zip > A2. The contents of the "A2" folder are displayed, including several subfolders (1, 2, 3, 4, 5) and an SDF file named "A2.nmredata.sdf". A context menu is open over the SDF file, showing options like "Properties of structure 1", "SDF Properties", and "Open with".

The right window shows the "Multi-Structure Viewer" application. It displays the SDF file "A2.nmredata.sdf" which contains one total structure. The structure is highlighted with a red border. The chemical structure is a cyclohexane derivative with a carbonyl group at position 1 and an amide group at position 4. A methyl group is also present. The chemical formula is labeled as  $C_{15}H_{23}NO_4$ . The molecular weight is listed as 281.34800 and the mono isotopic mass as 281.16271.

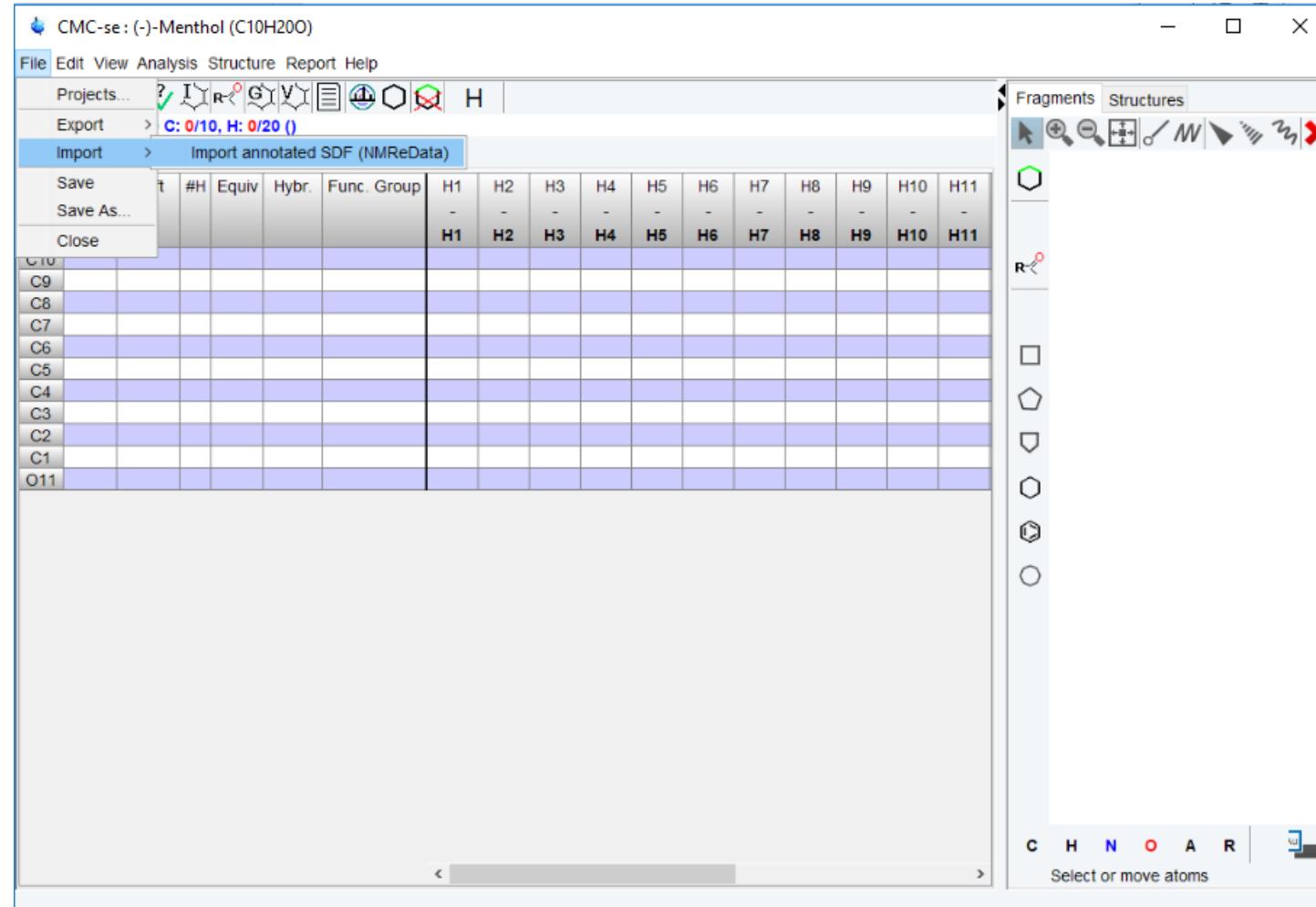
Properties of structure 1:

- Compound 1
- Formula =  $C_{15}H_{23}NO_4$
- Molecular weight = 281.34800
- Mono isotopic mass = 281.16271

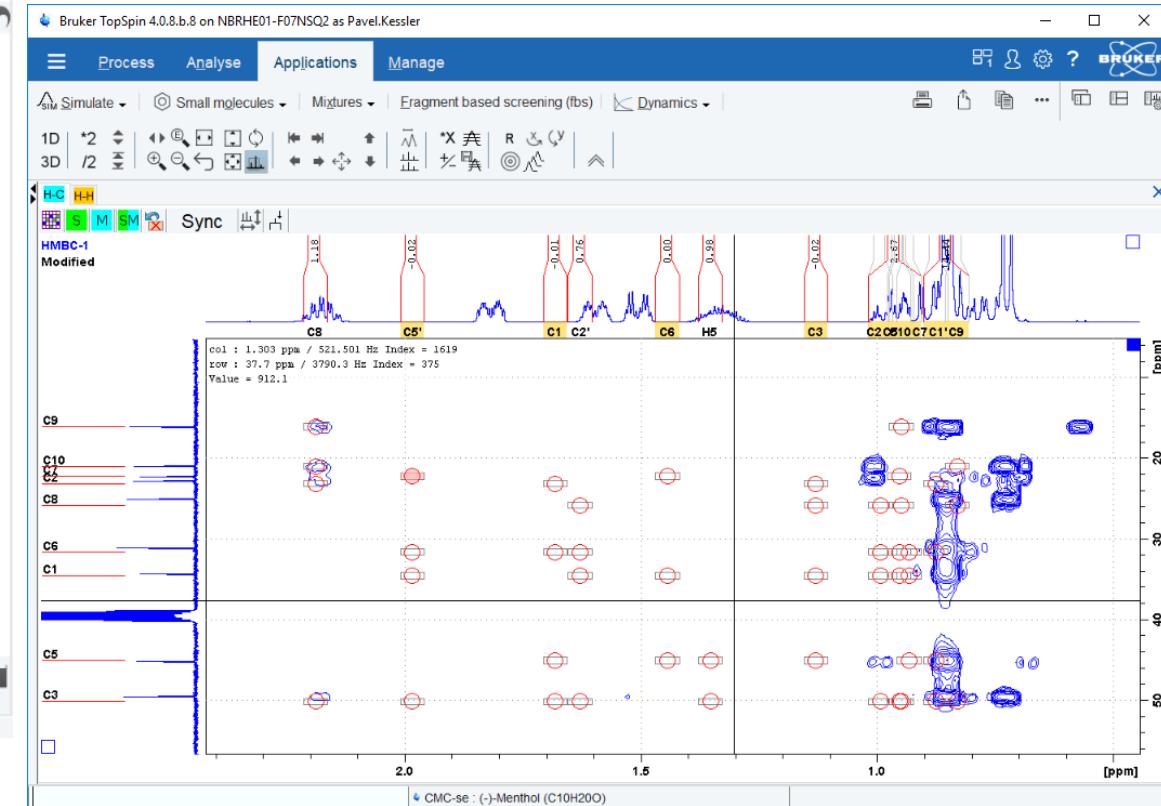
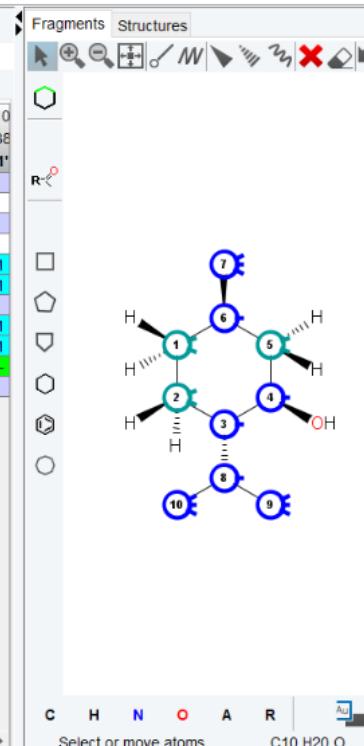
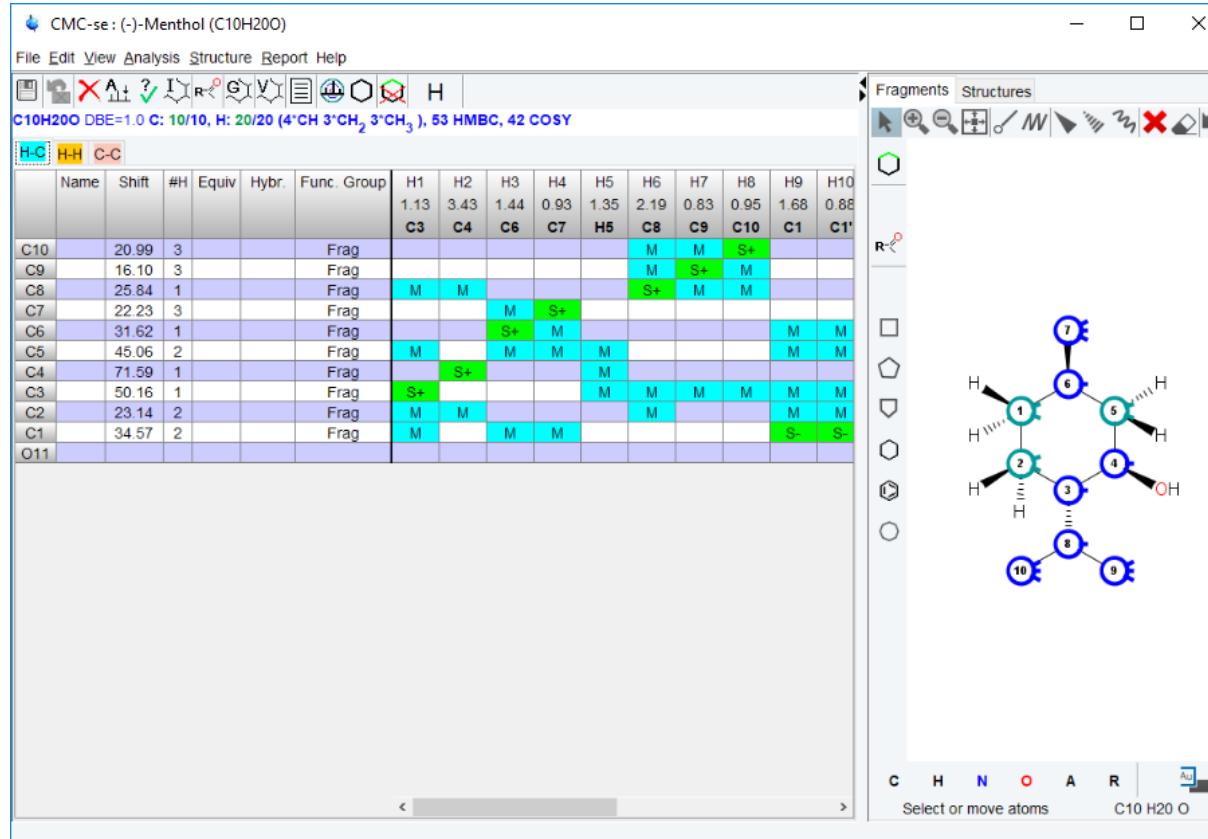
SDF Properties:

```
NMREDATA_LEVEL = 3
NMREDATA_CERTIFICATION = Software=CMC-se
NMREDATA_SOLVENT = DMSO
NMREDATA_FORMULA = C15H23NO4
NMREDATA_SMILES = C1(C(C(CC2CC(NC(C2)=O)=O)O)CC(C)CC1C)=O
NMREDATA_INCHI = InChI=1/C15H23NO4/c1-8-3-9(2)15(20)11(4-8)12(17)5-10-6-13(18)16-14(19)7-10/h8-12,17H,3-7H2,1-2H3,(H,16,18,19)/h16H
NMREDATA_TEMPERATURE = 298.0
NMREDATA_PH = 0.0
NMREDATA_ASSIGNMENT = c1, 214.103, 1\
c2, 173.990, 2\
c3, 173.829, 3\
c4, 65.354, 4\
c5, 50.995, 5\
c6, 42.762, 6\
c7, 40.720, 7\
```

# NMReData Import



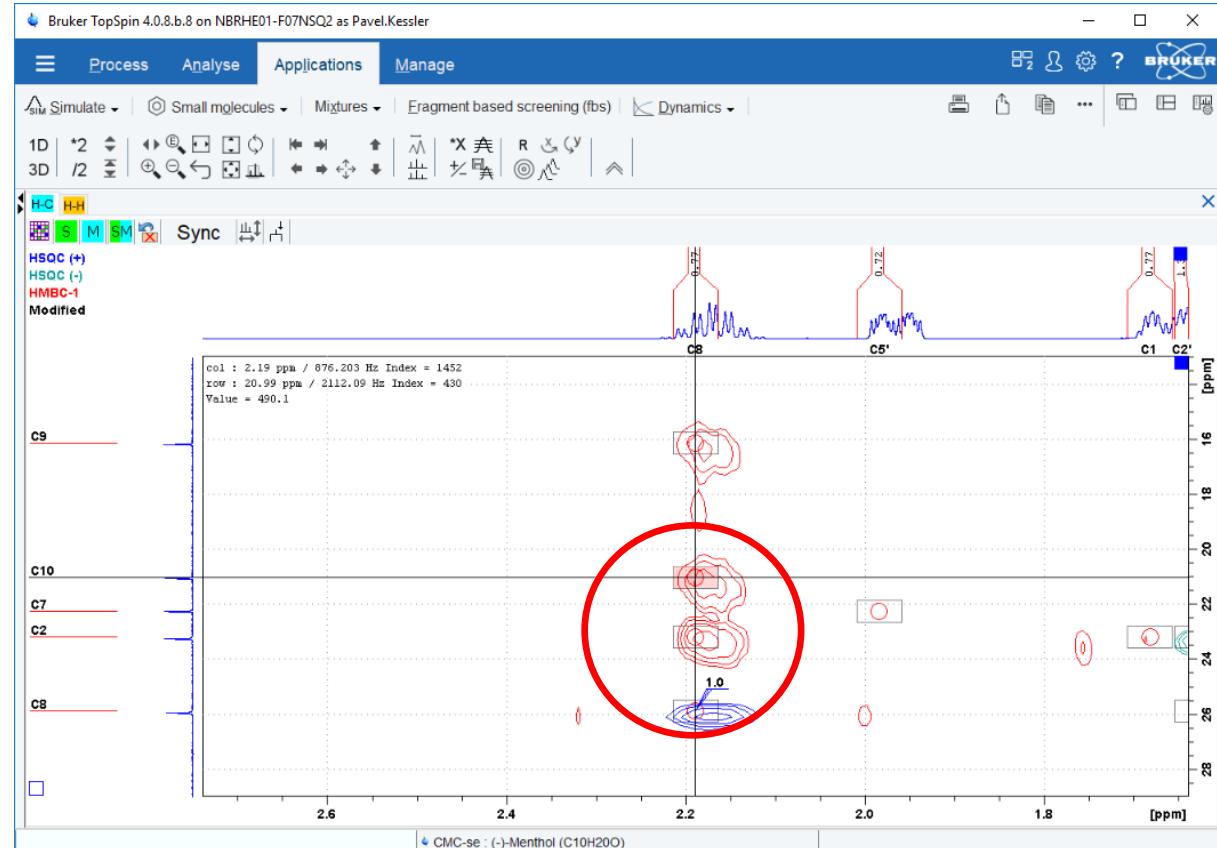
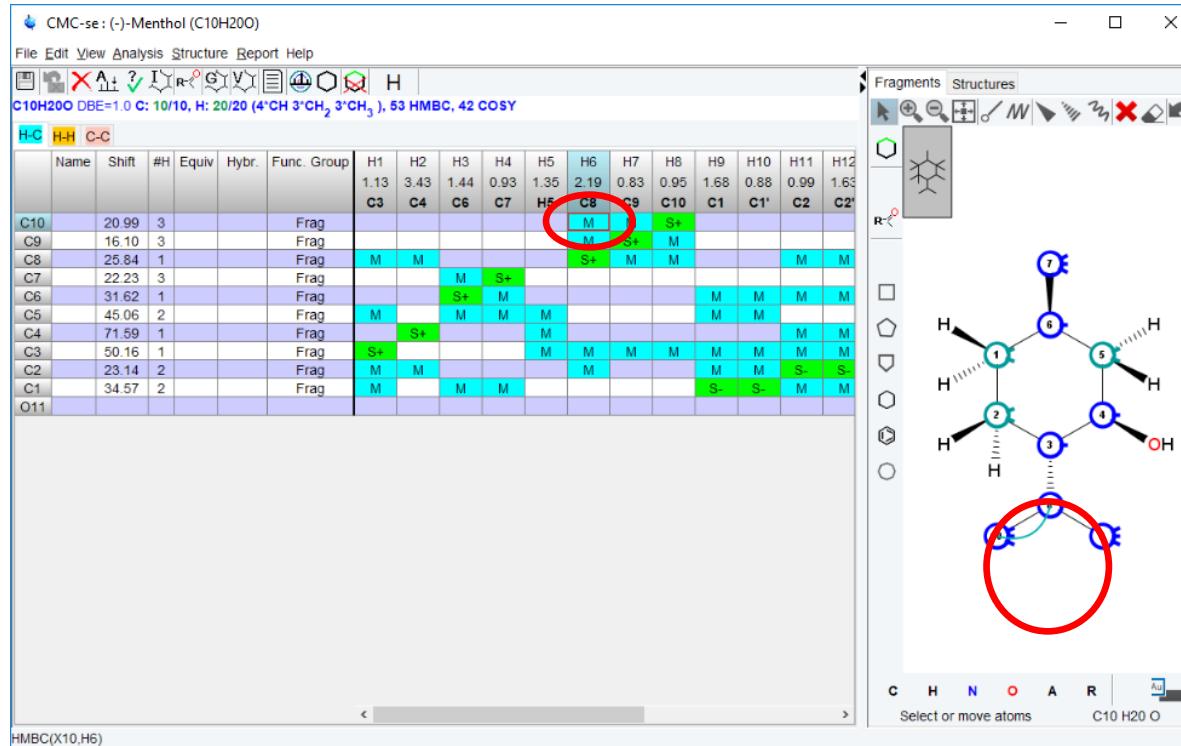
# NMReData Import



# NMReData Import



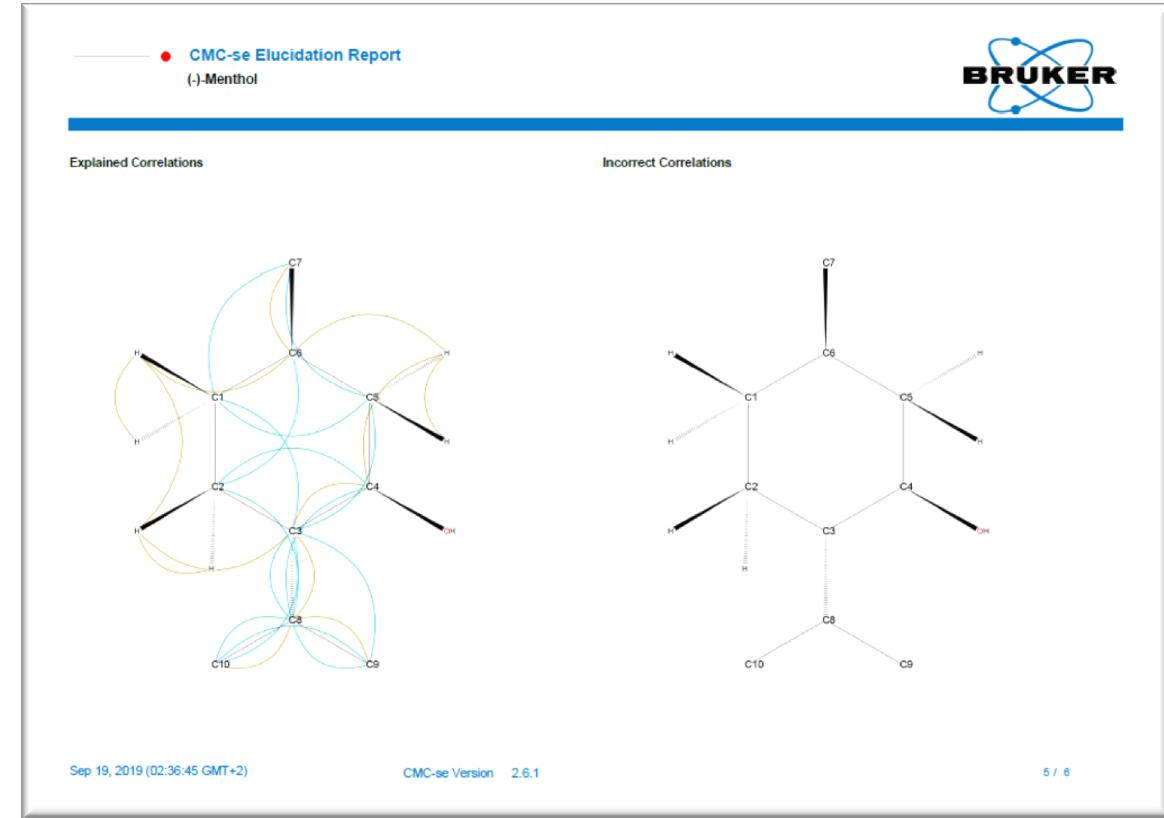
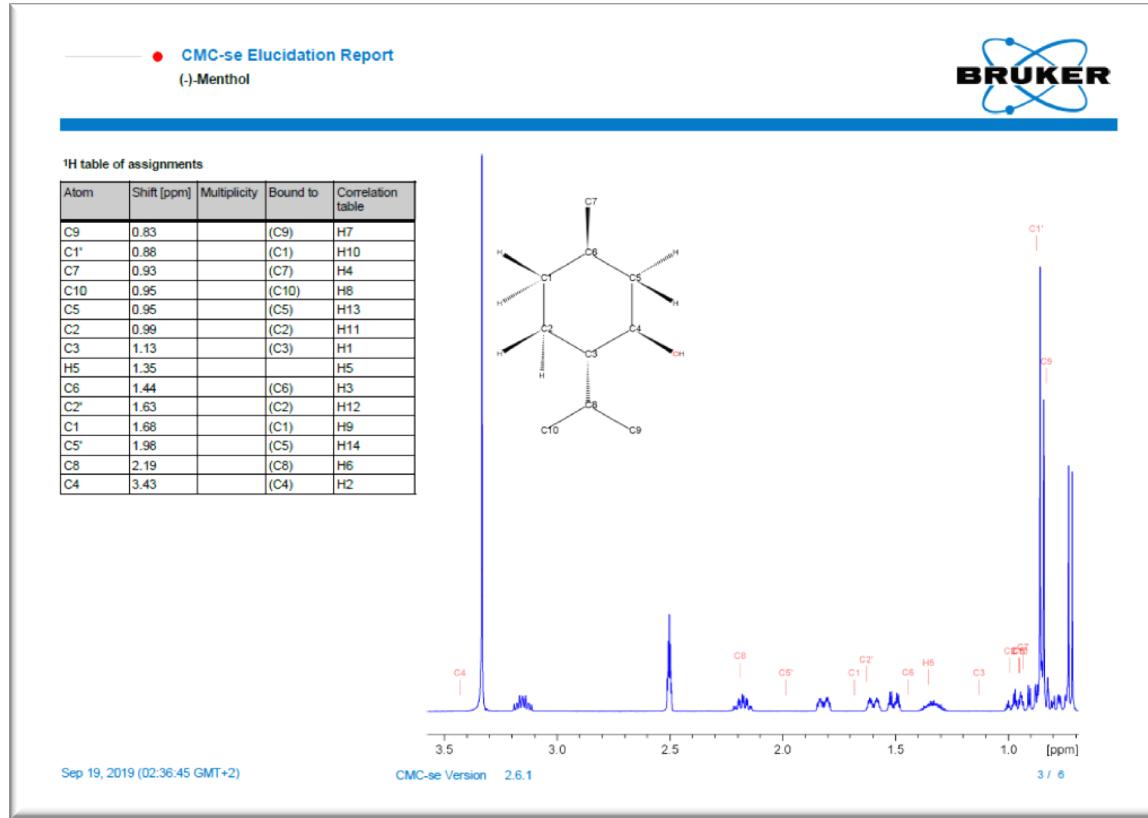
Detailed data inspection available



# NMReData Import



## Reporting



# NMReData Import



Beyond the data inspection: generate any structure proposals matching the data

CMC-se : (-)-Menthol (C<sub>10</sub>H<sub>20</sub>O)

File Edit View Analysis Structure Report Help

C<sub>10</sub>H<sub>20</sub>O DBE=1.0 C: 10/10, H: 20/20 (4°CH 3°CH<sub>2</sub> 3°CH<sub>3</sub>), 53 HMBC, 42 COSY

H-C H-H C-C

	Name	Shift	#H	Equiv	Hybr.	Func. Group	H1	H2	H3	H4	H5	H6	H7	H8	H9	H10	H11	H12	H13	H14	H15	H16	H17	H18	H19	H20		
C10		20.99	3			Frag						M	M	S+														
C9		16.10	3			Frag						M	S+	M														
C8		25.84	1			Frag	M	M				S+	M	M			M	M										
C7		22.23	3			Frag			M	S+							M	M	M	M	M	M	M					
C6		31.62	1			Frag			S+	M							M	M	M	M	M	M	M					
C5		45.06	2			Frag	M		M	M	M					M	M		S-	S-								
C4		71.59	1			Frag		S+				M					M	M	M	M	M	M	M					
C3		50.16	1			Frag	S+					M	M	M	M	M	M	M	M	M	M	M	M					
C2		23.14	2			Frag	M	M				M				M	M	S-	S-									
C1		34.57	2			Frag	M		M	M						S-	S-	M	M	M	M	M	M					
O11																												

Structure Generation Options

Structure generator: Bruker

Execution Control:

- Filter results (keep only best ones)
- Maximum number of generated structures (0=no limit)
- Terminate after this many seconds (0=no limit)
- Use multiple processors

Substructures:

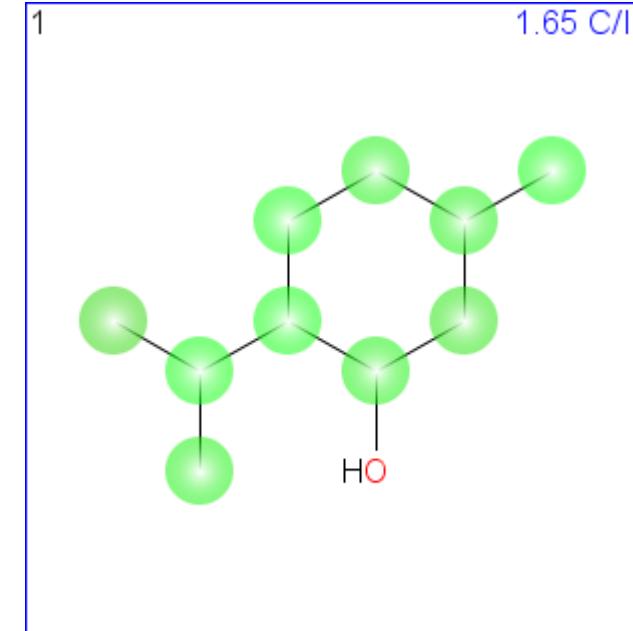
- Use defined substructures
- Ring rules
  - Structure does not contain any rings
  - Maximum ring length (0=no limit)
  - Forbidden rings lengths (Comma separated e.g. "3,4")
  - Required rings lengths (Comma separated e.g. "5,6")
  - Keep epoxides also if the cyclopropanes are forbidden

Correlations:

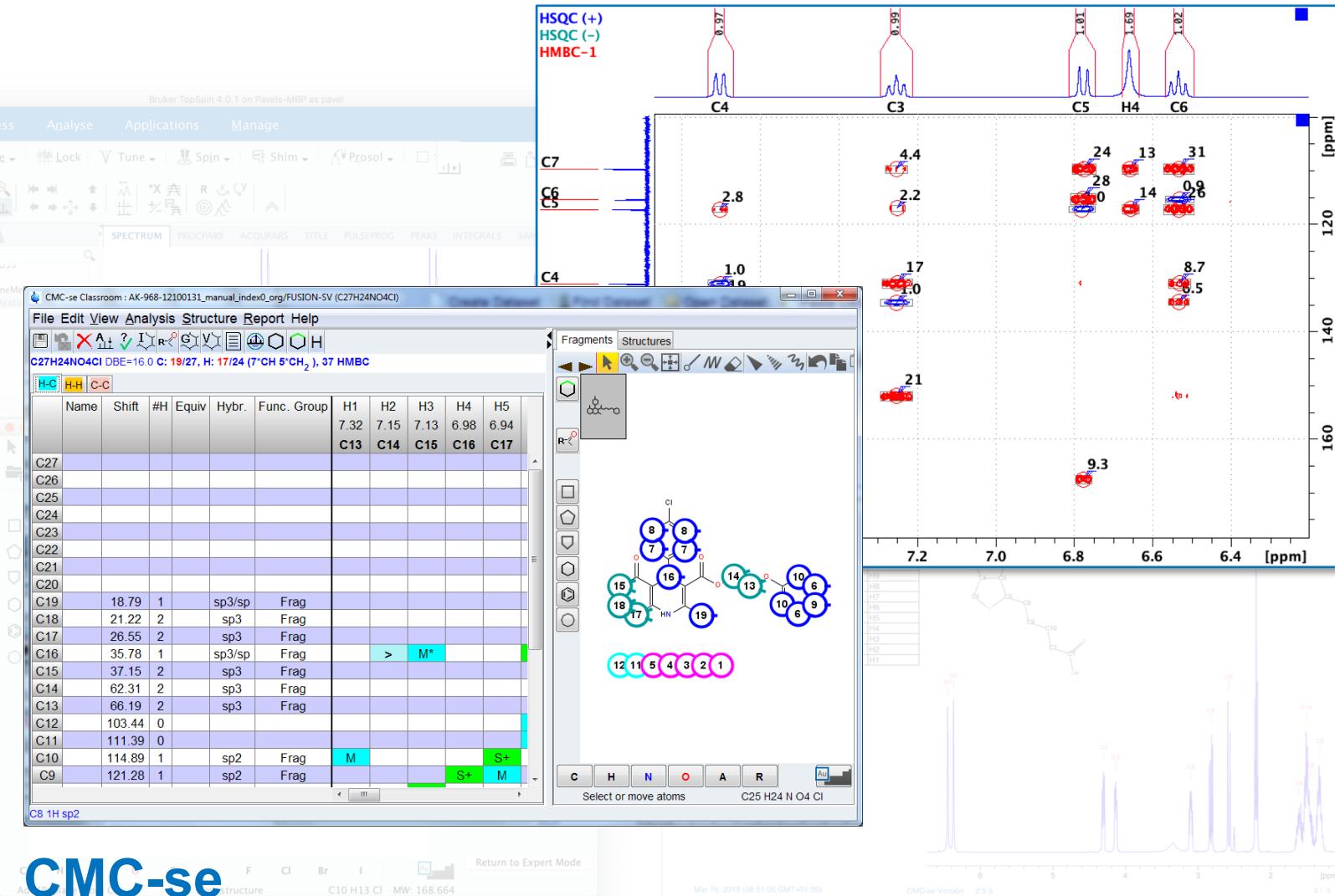
- Use COSY correlations
- Use HMBC correlations
- Auto-eliminate invalid or long range COSY correlations
- Auto-eliminate invalid or long range HMBC correlations
- Maximum number of eliminated correlations (COSY+HMBC)
- HMBC/COSY autoelimination policy: Optimal

Chemistry rules

Generate Structures Cancel



# NMReData Implementation Availability



# CMC-se: Classroom Edition



## CMC-se: Classroom Edition

- Peak picking
- Number of attached protons
- Filling correlation table
- Displays correlations of each atom
- Manually builds up structure
- Editable basic NMR lecture
- Example datasets for use with CMC-se
- Requires a license

The license is free and included in the  
Topspin license for academia

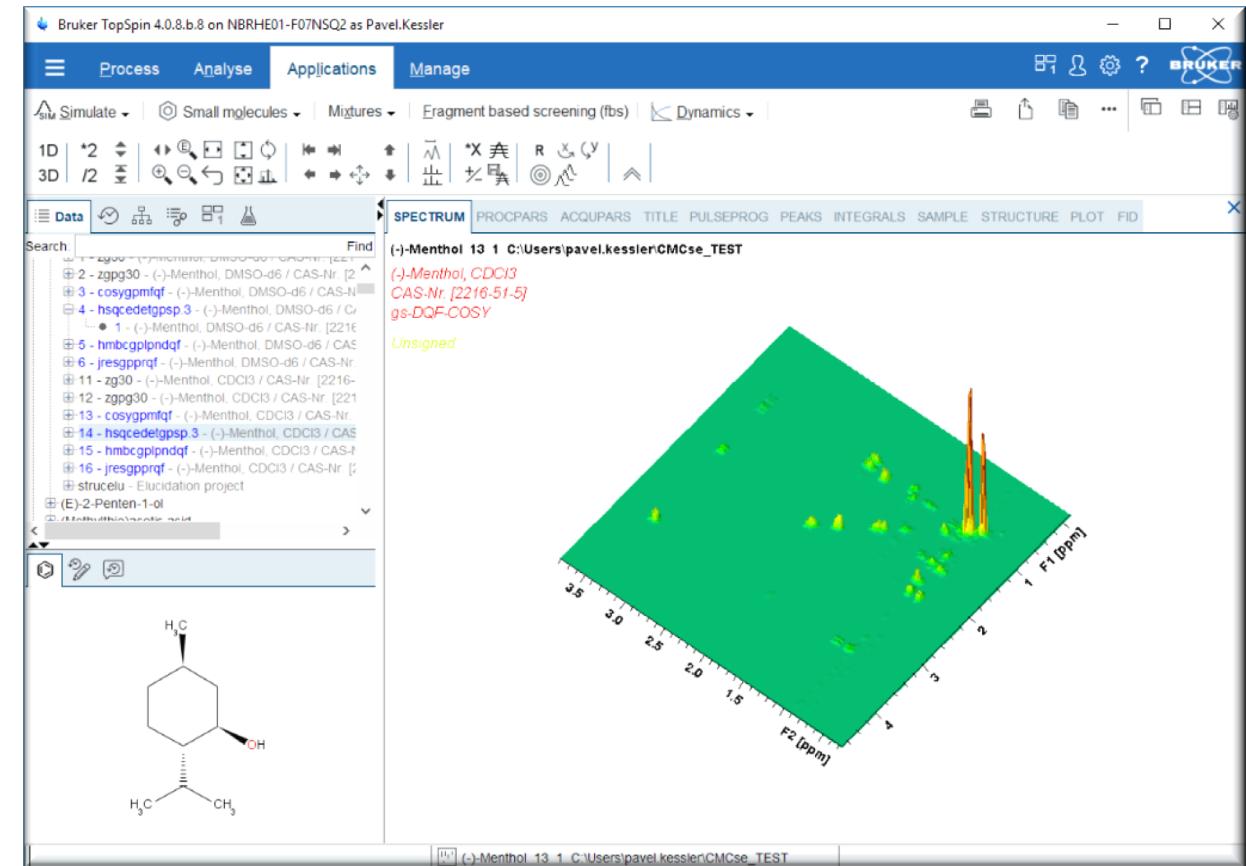
- **Structure generator**

# NMReData Implementation Availability



- implemented in CMC-se
- Import - Topspin 4.\* and Topspin 3.6.1
- Export - Topspin 4.0.8
- Included also in CMC-se ClassRoom Edition

- Topspin processing license is free for academia
- CMC-se ClassRoom edition is included since March 2019
- NMReData implementation is free for academic customers



# NMReData Quo Vadis ?



- Reference data and validation tests for developer
- Cleanup the format definition

```
> <NMREDATA_2D_13C_NJ_1H>
Larmor=400.150\
CorType=HMBC\
Spectrum_Location=file:/Users/pavel/CMCse_TEST/2,4-Dimethoxybenzylalkohol/15/pdata/1 \
Pulseprogram=hmbcgplpndqf\
...
c1/ (h3, h2) , E=7.23121e+06, W2=30.52, W1=203.42\
c1/ (h3 | h2) , E=7.23121e+06, W2=30.52, W1=203.42\
```

- Consistency checks
  - Signatures, detect modifications
- Involve additional partners
  - JCamp, NMRml
  - Allotrope foundation



Thank you!