

Bruker NMReData Implementation

NMReData Meeting, Porto 2019

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Bruker BioSpin



Outline

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



NMReData Export



CMC-se

- Structure elucidation
- Structure validation

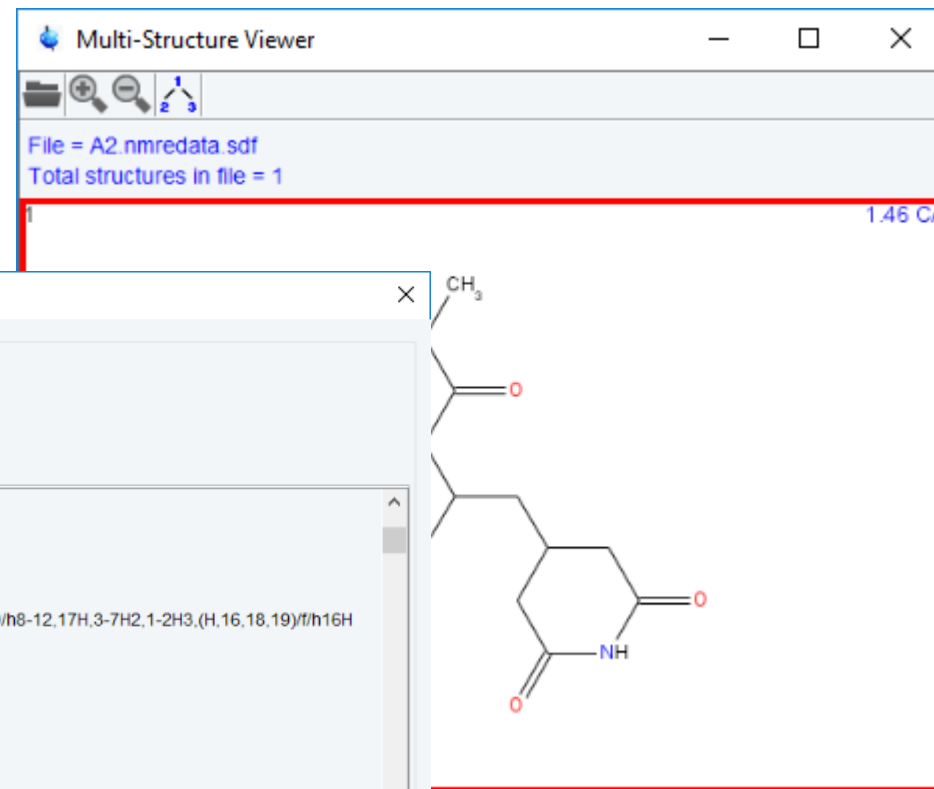
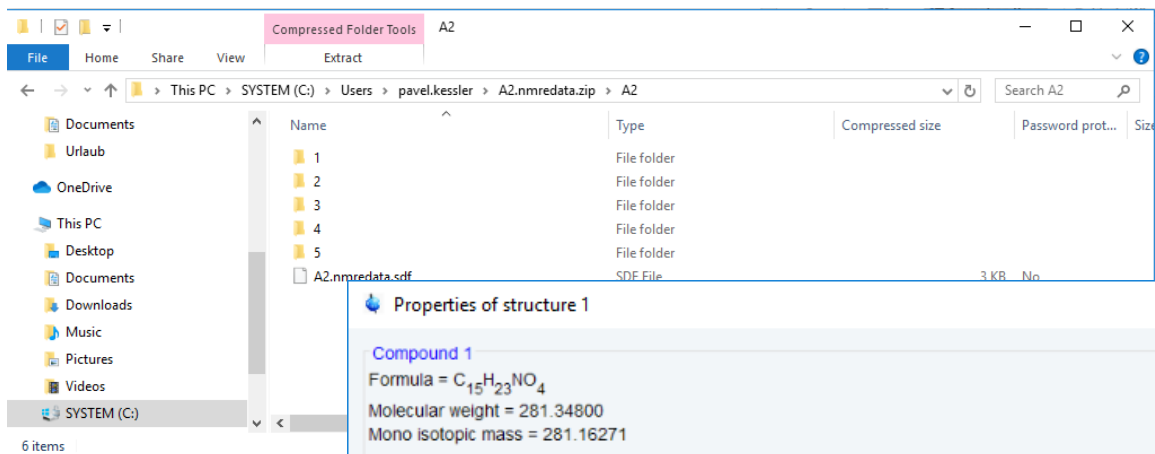
The screenshot displays the Bruker software interface for NMR data analysis. The main window shows a table of NMR records with columns for chemical shift (ppm) and various coupling constants (J values). The table is titled "CMC-se: A2 (C15H23NO4)" and contains 15 rows of data. The columns are labeled H1 through H15, with corresponding chemical shifts and coupling constants. The table is color-coded with blue, green, and red cells.

Overlaid on the main window are three dialog boxes:

- NMR Records Export:** A dialog box for exporting NMR records. It includes fields for "NMR Records Destination Folder" (set to C:\Users\pavel.kessler) and "Comment".
- NMR Records:** A small information dialog box stating "CMC-se project was exported to C:\Users\pavel.kessler\A2.nmredata.zip".
- Chemical Structure:** A chemical structure diagram of a complex molecule, likely a sugar derivative, with atoms numbered 1 through 15. The structure is shown in a 3D perspective view.

	#H	Equiv	Hybr.	Func. Group	H1	H2	H3	H4	H5	H6	H7	H8	H9	H10	H11	H12	H13	H14	H15
C15	15.01	3	sp3		10.55	4.29	3.70	2.49	2.45	2.36	2.33	2.14	2.13	2.10	1.95	1.83	1.67	1.4	
C14	18.69	3	sp3		H1	H2	C4	C8	C10	C9	C5	C9'	C10'	C12	C13	C11	C6	C1	
	1		sp3/sp					M*	<								M		
	1		sp3/sp				M					>	M*	S+	<		M	M	M
	2		sp3				M			>	M*					S-	M	S	
	2		sp3		M			S-	M*	<	M*	S-	<	<					
	2		sp3		M			M	S		S-	>	M*	<					
	1		sp3/sp			v	v	S+										M	
	2		sp3		M*	M*											M	S-	M
	2		sp3		M	M		M*	<								M	S-	M
	1		sp3/sp		M	M	S+			>	M*						M		M
					M*				M*										
					^				^										

NMReData Export



Properties of structure 1

Compound 1
Formula = C₁₅H₂₃NO₄
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)/t16H
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\
```

OK

NMReData Import



CMC-se: (-)-Menthol (C10H20O)

File Edit View Analysis Structure Report Help

Projects... H

Export > C: 0/10, H: 0/20 ()

Import > Import annotated SDF (NMReData)

Save Save As... Close

	#H	Equiv	Hybr.	Func. Group	H1	H2	H3	H4	H5	H6	H7	H8	H9	H10	H11
					H1	H2	H3	H4	H5	H6	H7	H8	H9	H10	H11
C10															
C9															
C8															
C7															
C6															
C5															
C4															
C3															
C2															
C1															
O11															

Fragment Structures

C H N O A R

Select or move atoms

NMReData Import



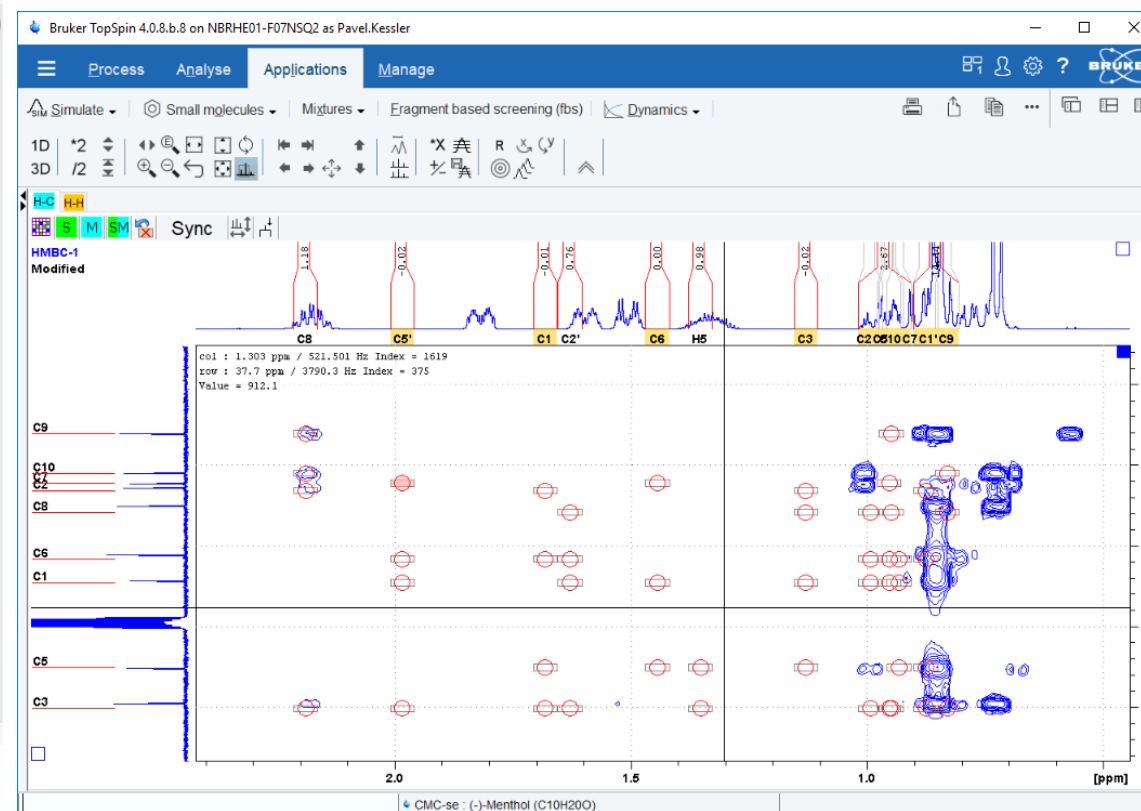
CMC-se: (-)-Menthol (C10H20O)

File Edit View Analysis Structure Report Help

C10H20O DBE=1.0 C: 10/10, H: 20/20 (4*CH 3*CH₂ 3*CH₃), 53 HMBC, 42 COSY

	Name	Shift	#H	Equiv	Hybr.	Func. Group	H									
							H1	H2	H3	H4	H5	H6	H7	H8	H9	H10
							C3	C4	C6	C7	H5	C8	C9	C10	C1	C1'
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		
C7		22.23	3			Frag			M	S+						
C6		31.62	1			Frag			S+	M					M	M
C5		45.06	2			Frag	M			M	M				M	M
C4		71.59	1			Frag		S+			M					
C3		50.16	1			Frag	S+				M	M	M	M	M	M
C2		23.14	2			Frag	M	M			M				M	M
C1		34.57	2			Frag	M		M	M					S-	S-
O11																

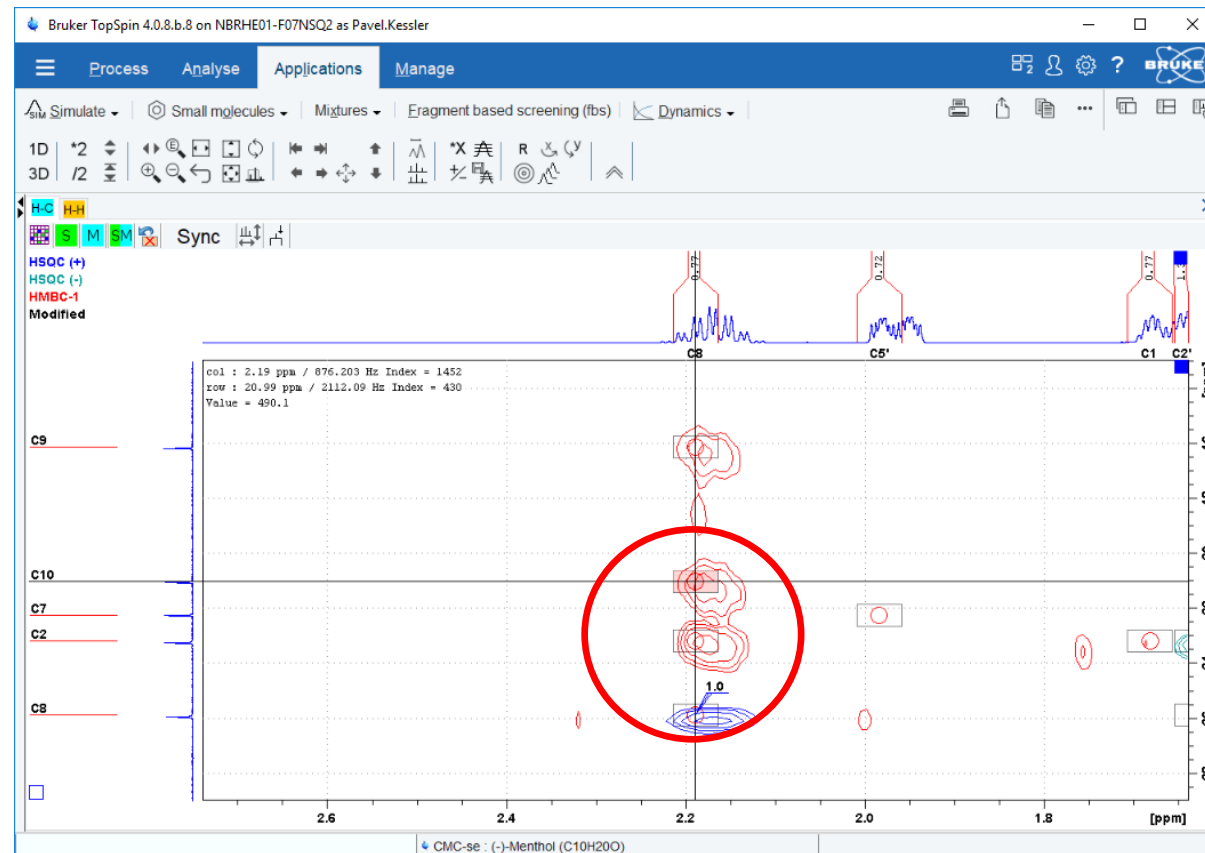
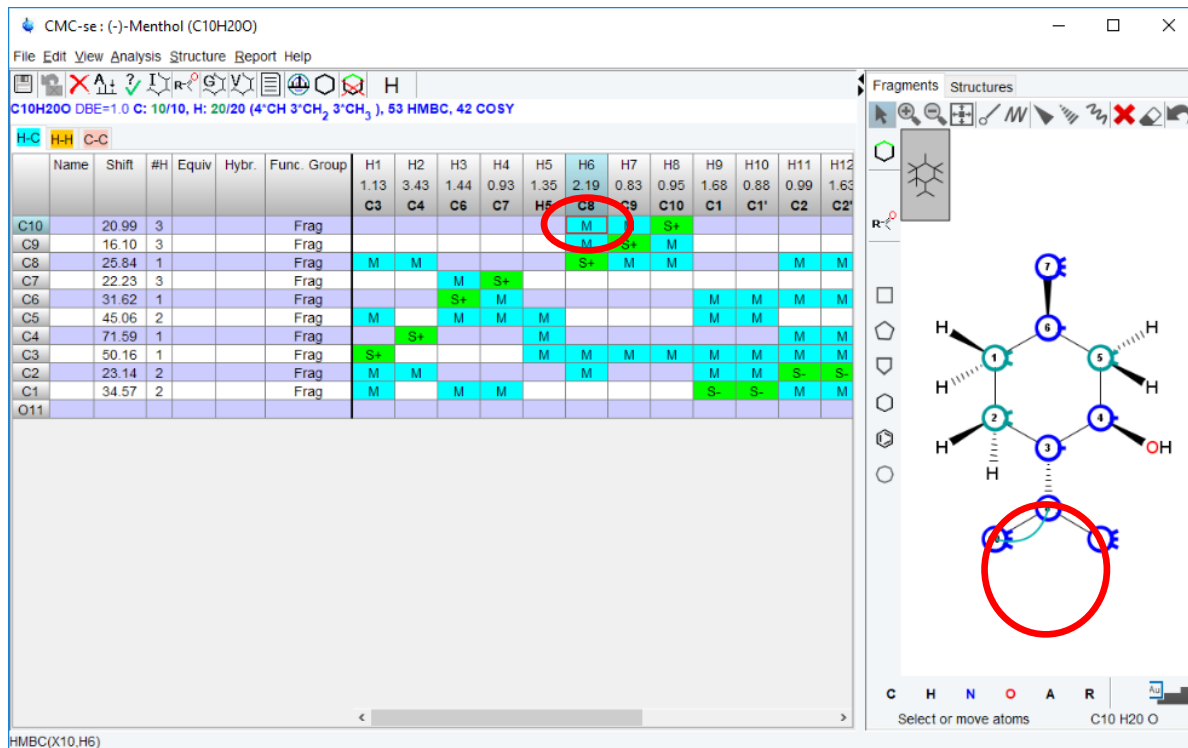
Select or move atoms C10 H20 O



NMReData Import

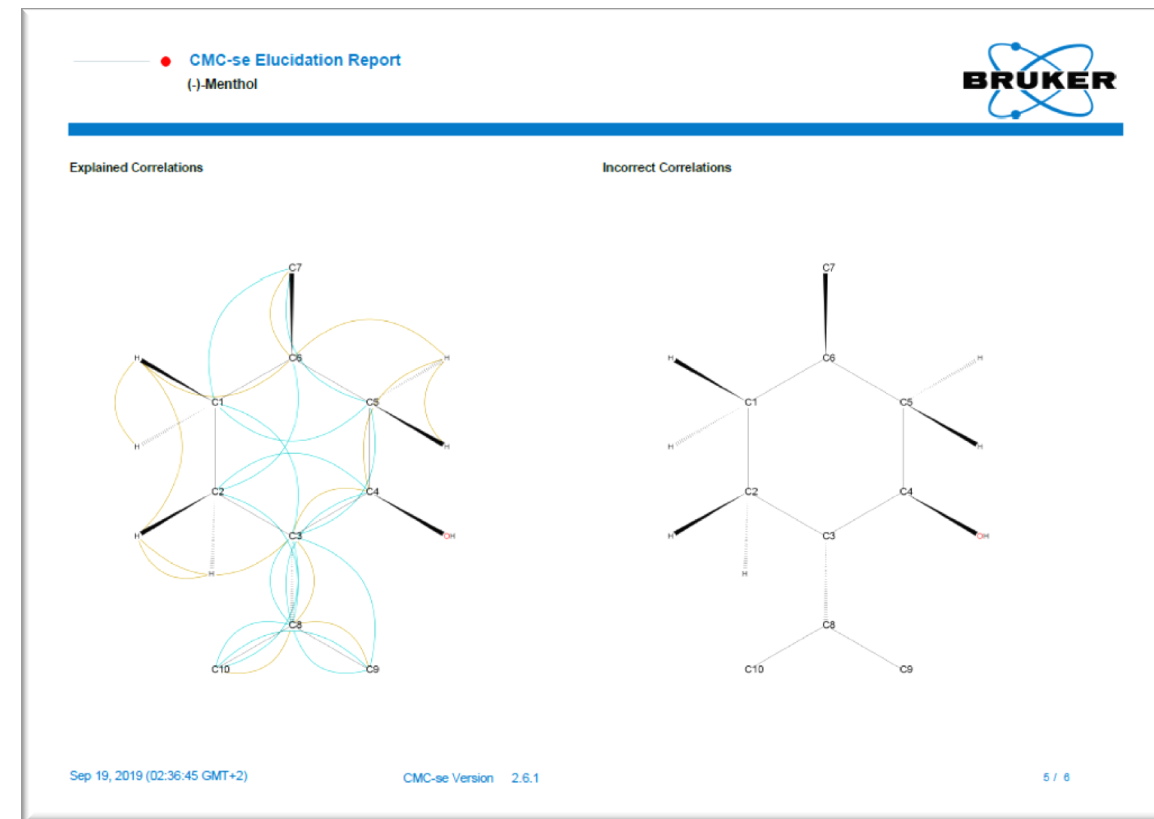
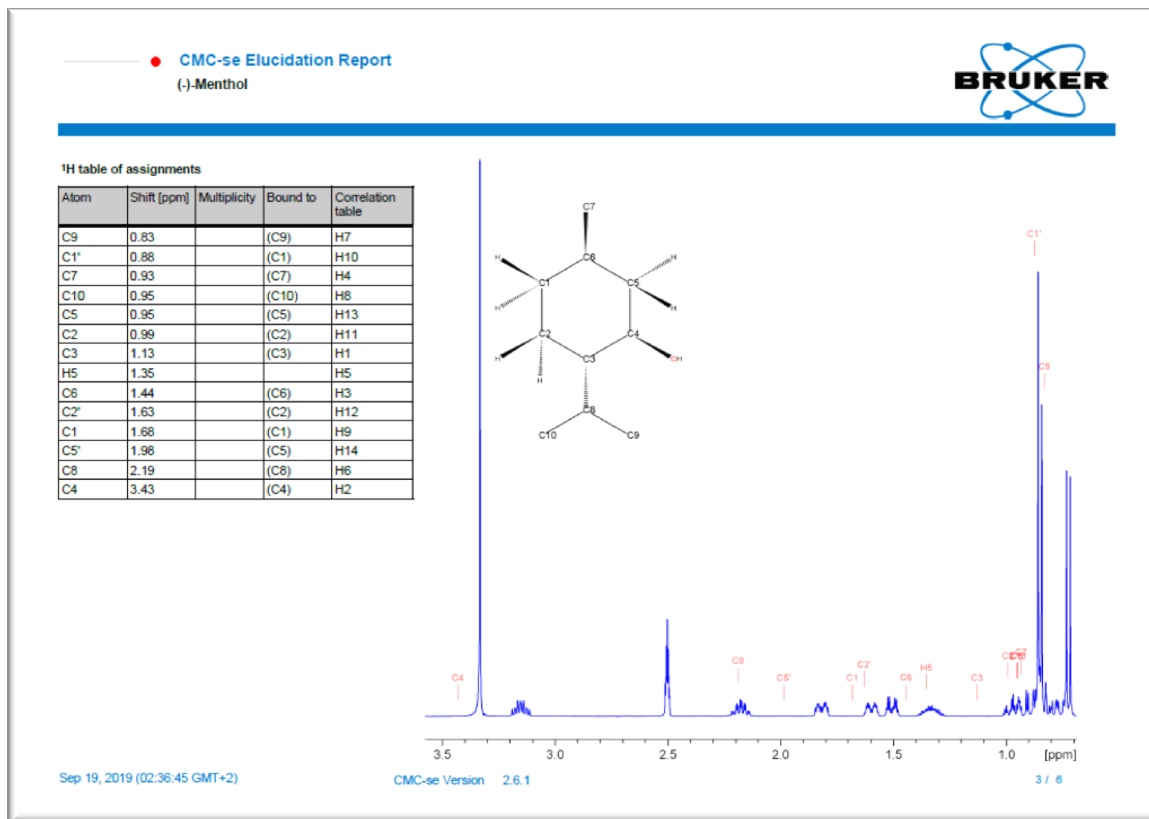


Detailed data inspection available



NMReData Import

Reporting



NMReData Import



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

CMC-se: (-)-Menthol (C10H20O)

File Edit View Analysis Structure Report Help

C10H20O DBE=1.0 C: 10/10, H: 20/20 (4^oCH 3^oCH₂ 3^oCH₃), 53 HMBC, 42 COSY

H-C H-H C-C

	Name	Shift	#H	Equiv	Hybr.	Func. Group	H1 1.13 C3	H2 3.43 C4	H3 1.44 C6	H4 0.93 C7	H5 1.35 H5	H6 2.19 C8	H7 0.83 C9	H8 0.95 C10	H9 1.68 C1	H10 0.88 C1'	H11 0.99 C2	H12 1.63 C2'	H13 0.95 C5	H14 1.98 C5'		
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		
C6		31.62	1			Frag			S+	M						M	M	M	M	M	M	
C5		45.06	2			Frag	M		M	M					M	M			S-	S-		
C4		71.59	1			Frag		S+			M							M	M	M	M	
C3		50.16	1			Frag	S+				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	
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

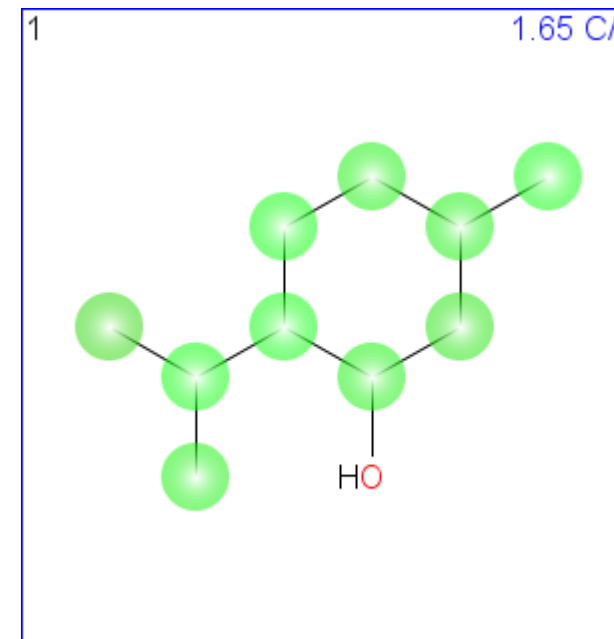
- Use defined substructures
- Ring rules
- Structure does not contain any rings
- Maximum ring length (0=no limit)
- Forbidden rings lengths (Comma separated e.g. "3,4")
- Required rings lengths (Comma separated e.g. "5,6")
- Keep epoxydes also if the cyclopropanes are forbidden

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

Chemistry rules

Generate Structures Cancel



NMReData Implementation Availability



Classroom

Brucker TopSpin 4.0.1 on Pavels-MBP as pavels

Process Analyse Applications Manage

Sample Lock Tune Spin Shim Prosol

SPECTRUM PROCPARS ACQPARS TITLE PULSEPROG PEAKS INTEGRALS SAS

CMC-se Classroom : AK-968-12100131_manual_index0.org/FUSION-SV (C27H24NO4Cl)

File Edit View Analysis Structure Report Help

C27H24NO4Cl DBE=16.0 C: 19/27, H: 17/24 (7*CH 5*CH₂), 37 HMBC

	Name	Shift	#H	Equiv	Hybr.	Func. Group	H1	H2	H3	H4	H5
							C13	C14	C15	C16	C17
C27											
C26											
C25											
C24											
C23											
C22											
C21											
C20											
C19		18.79	1		sp3/sp	Frag					
C18		21.22	2		sp3	Frag					
C17		26.55	2		sp3	Frag					
C16		35.78	1		sp3/sp	Frag			M*		
C15		37.15	2		sp3	Frag					
C14		62.31	2		sp3	Frag					
C13		66.19	2		sp3	Frag					
C12		103.44	0								
C11		111.39	0								
C10		114.89	1		sp2	Frag	M			S+	
C9		121.28	1		sp2	Frag			S+	M	

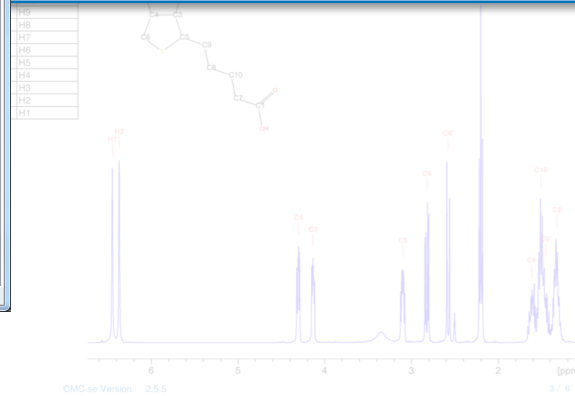
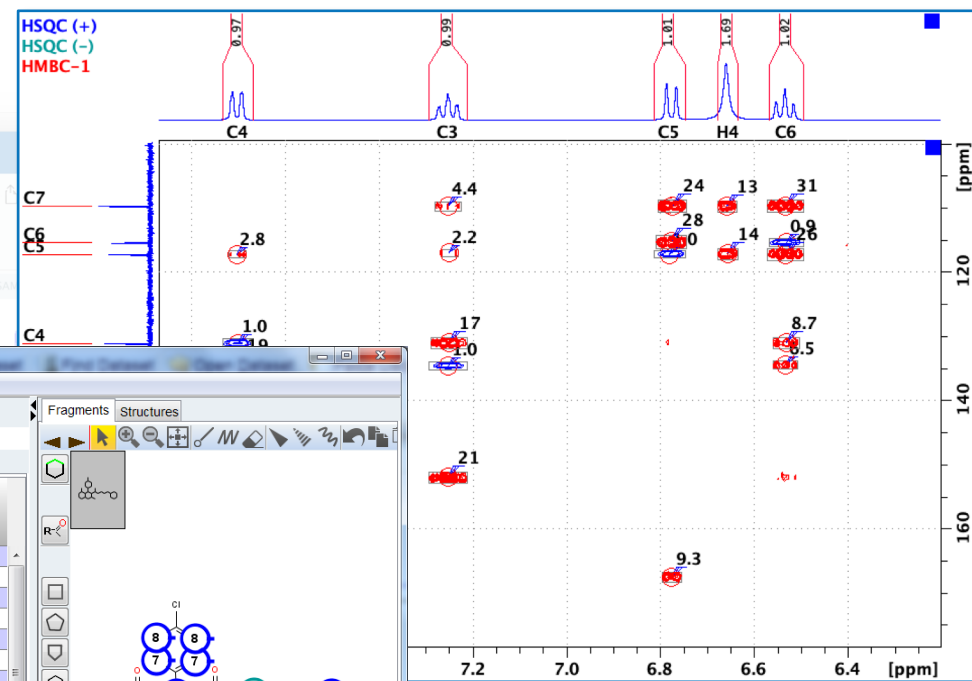
C8 1H sp2

Structure C10 H13 Cl MW: 168.664

Return to Expert Mode

Mar 16, 2016 09:51:05 GMT+01:00

CMC-se Version 3.5.5



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

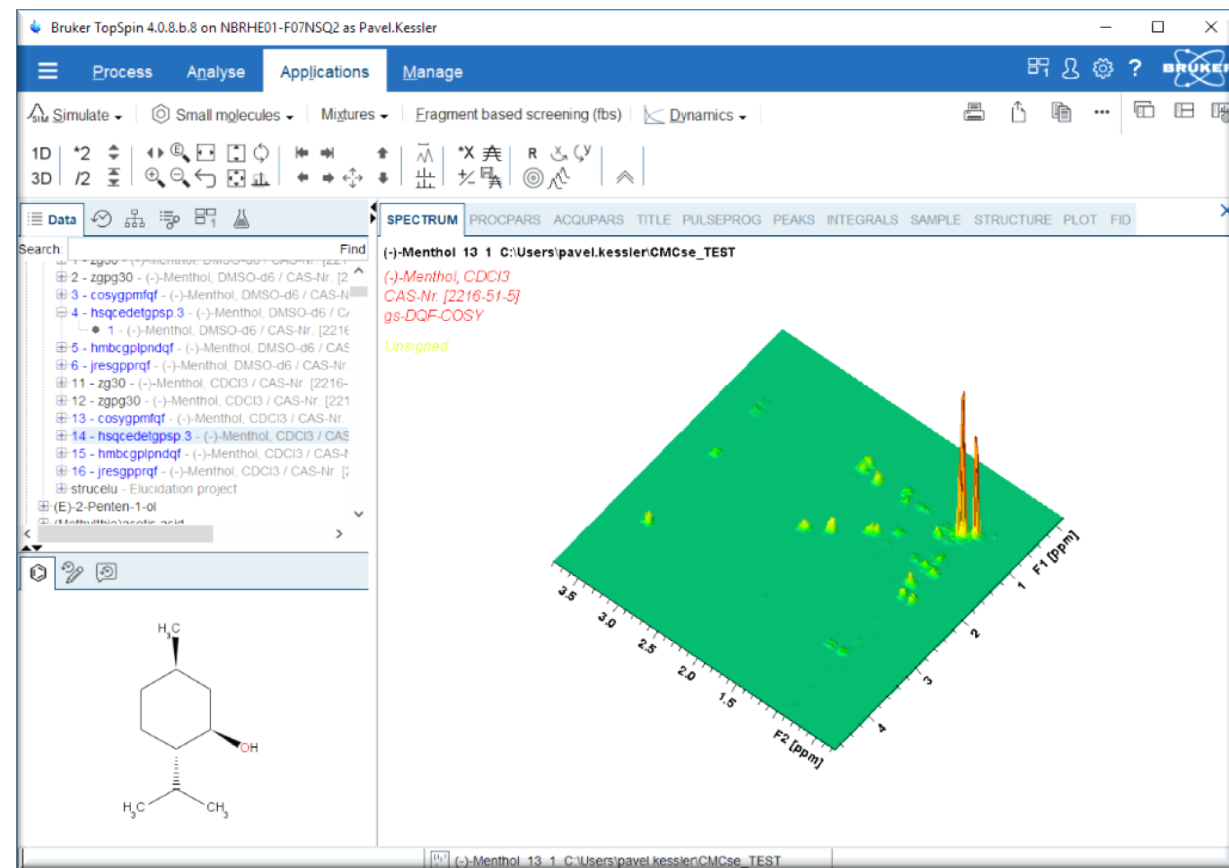
- ~~Structure generator~~

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=hmbcgp1pndqf\
...
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!