Bruker NMReData Implementation

NMReData Meeting, Porto 2019

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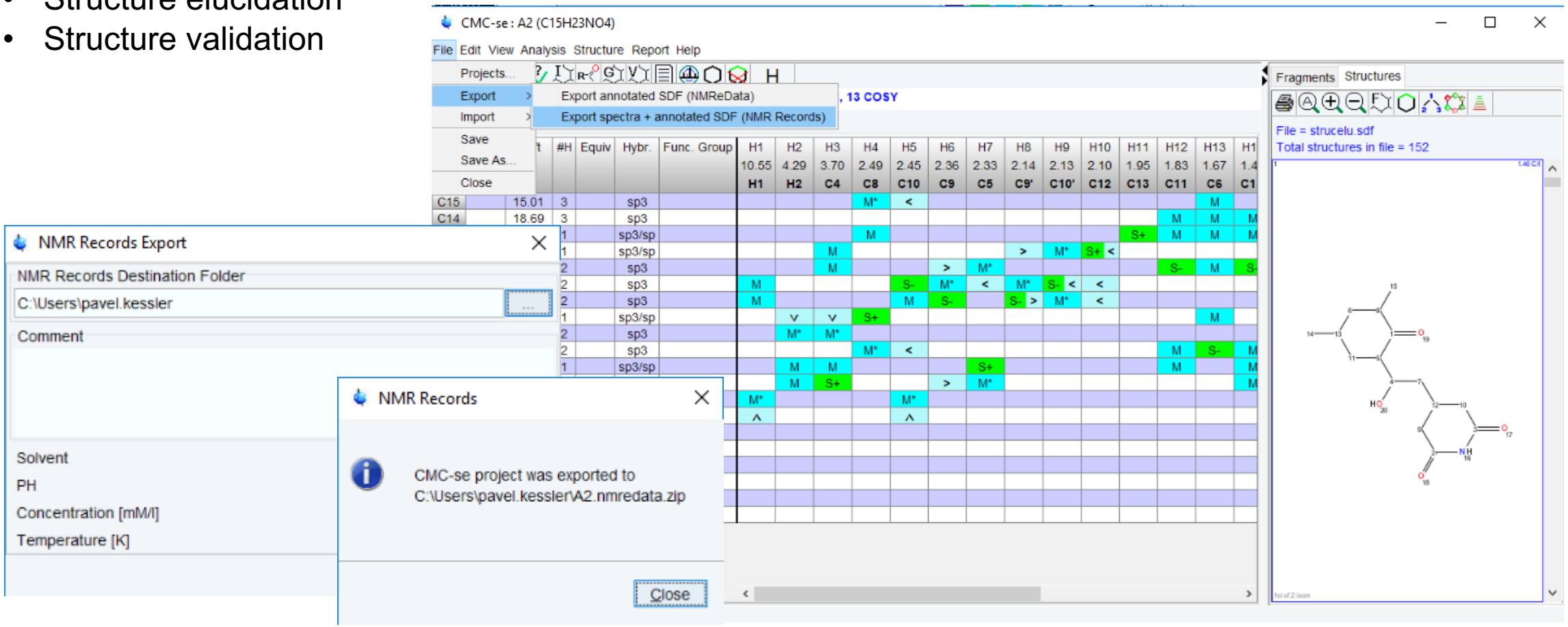
Bruker BioSpin

Outline

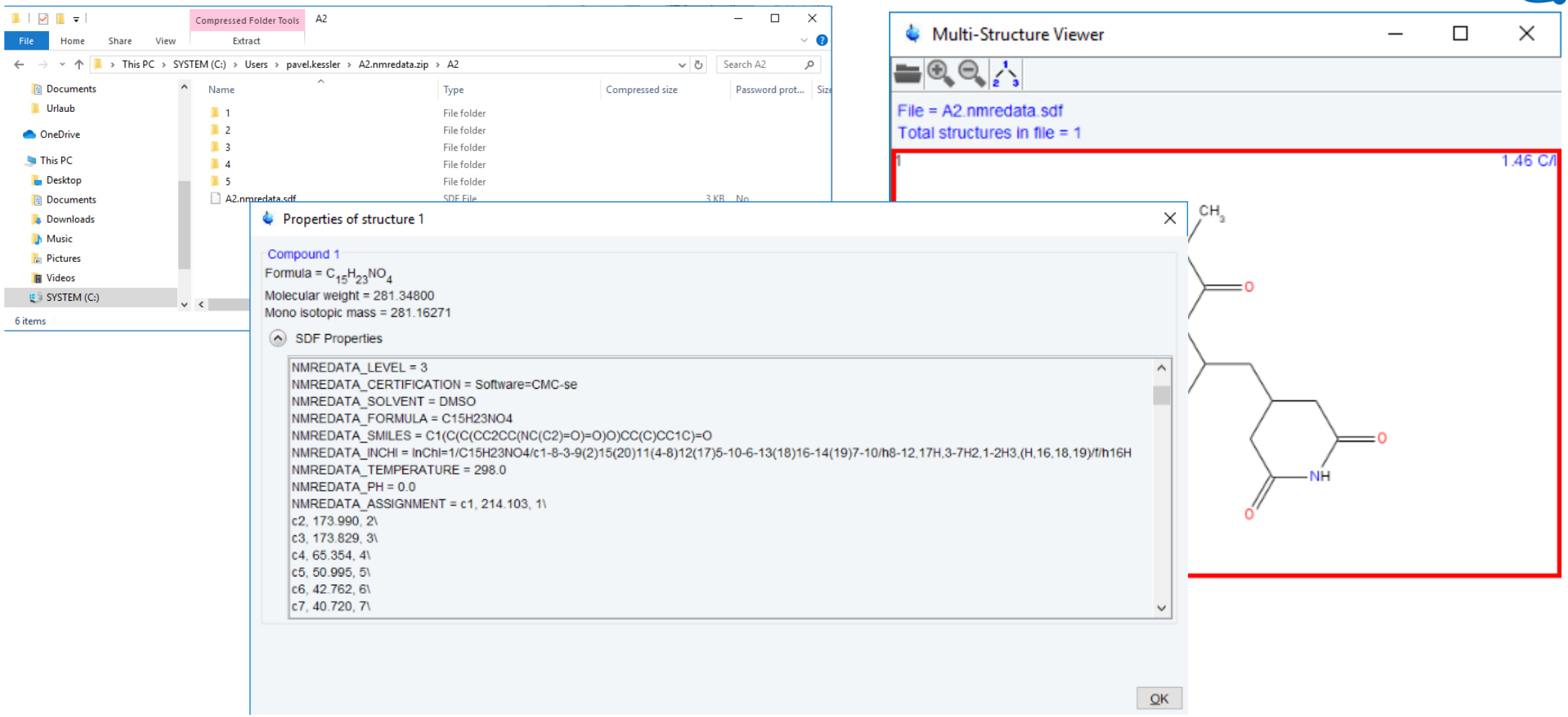
- NMReData and NMR Records export
- NMReData import
- Availability
- Technical comments

NMReData Export

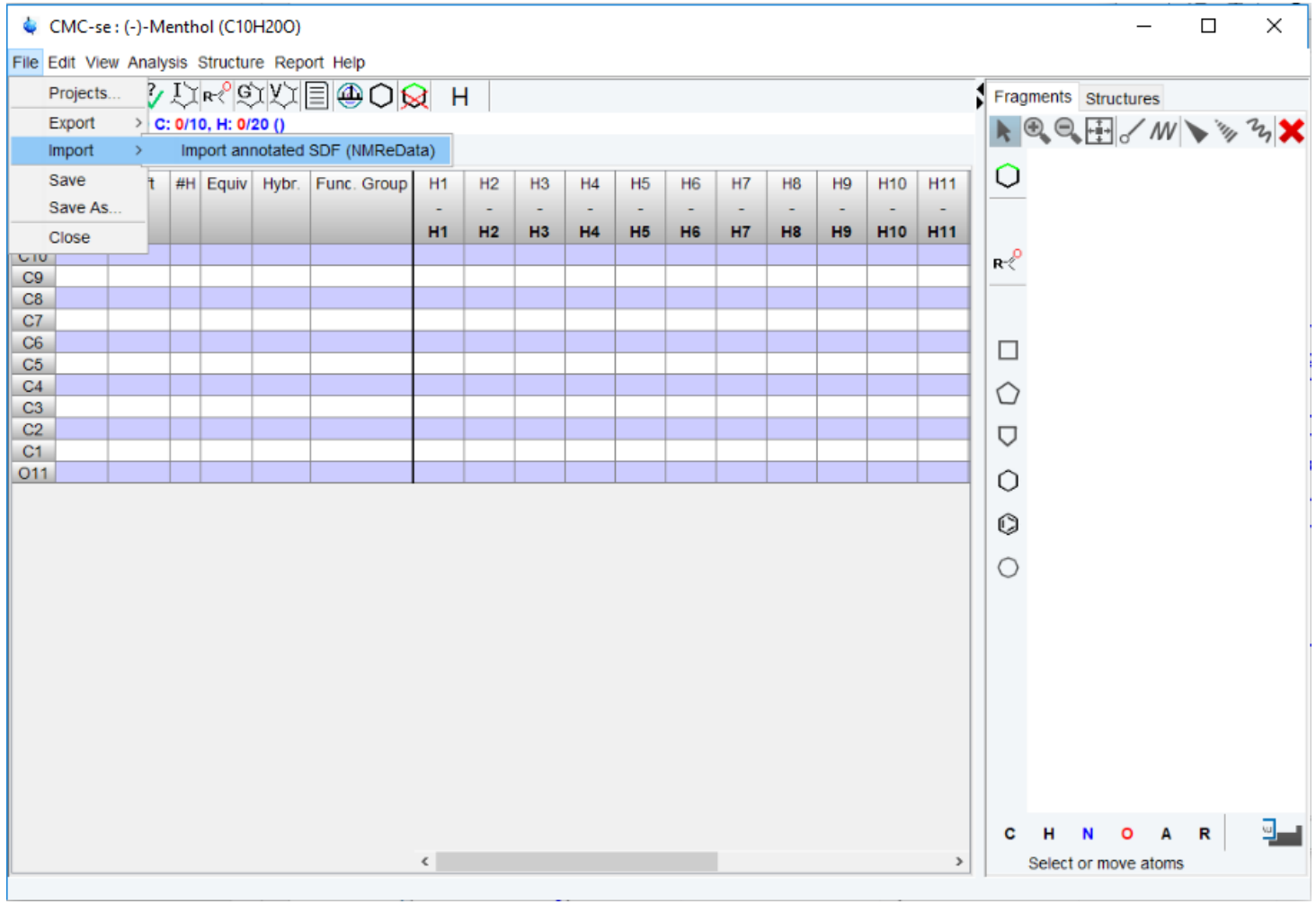
CMC-se
- Structure elucidation
- Structure validation



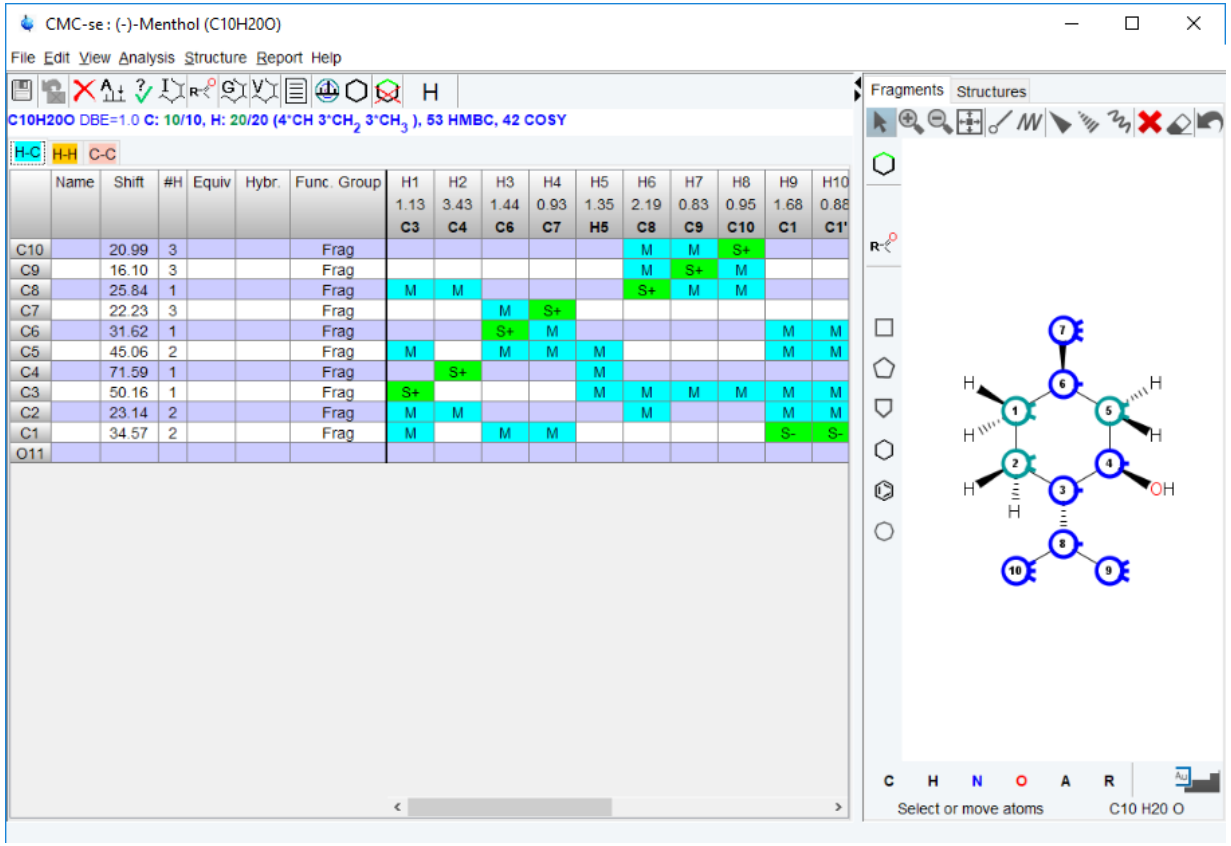
NMReData Export

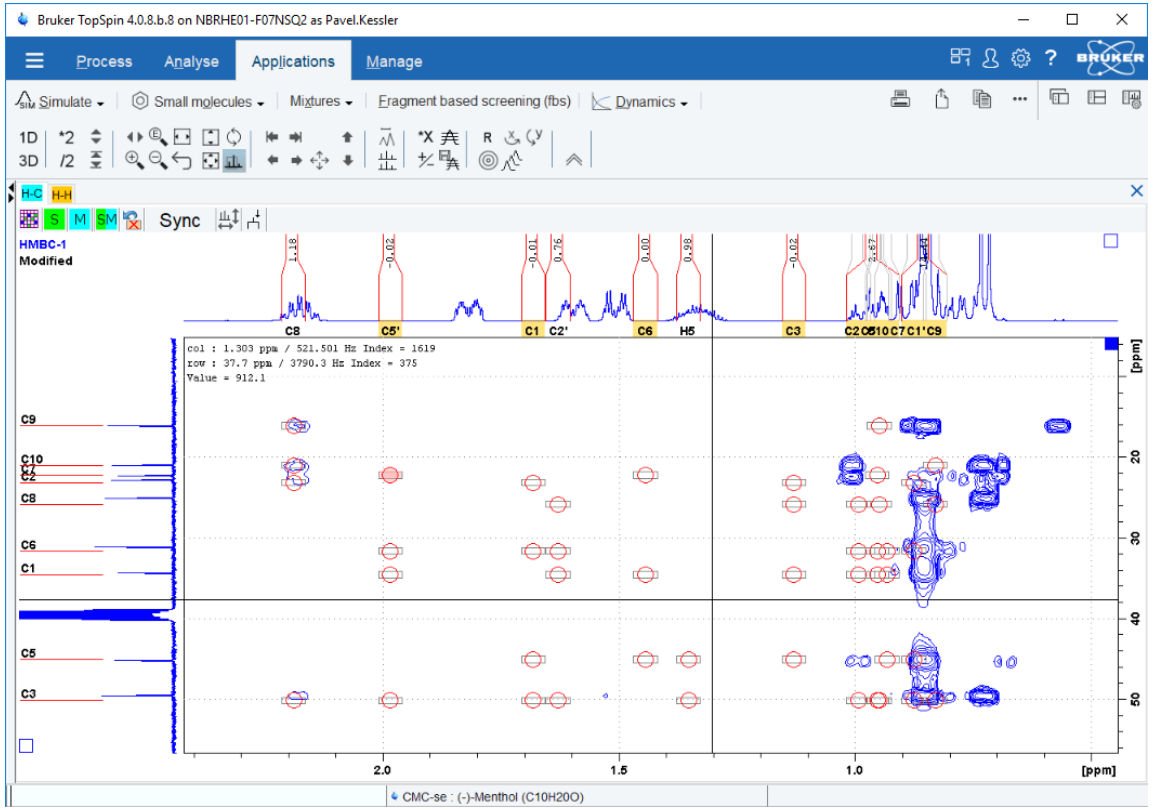


NMReData Import



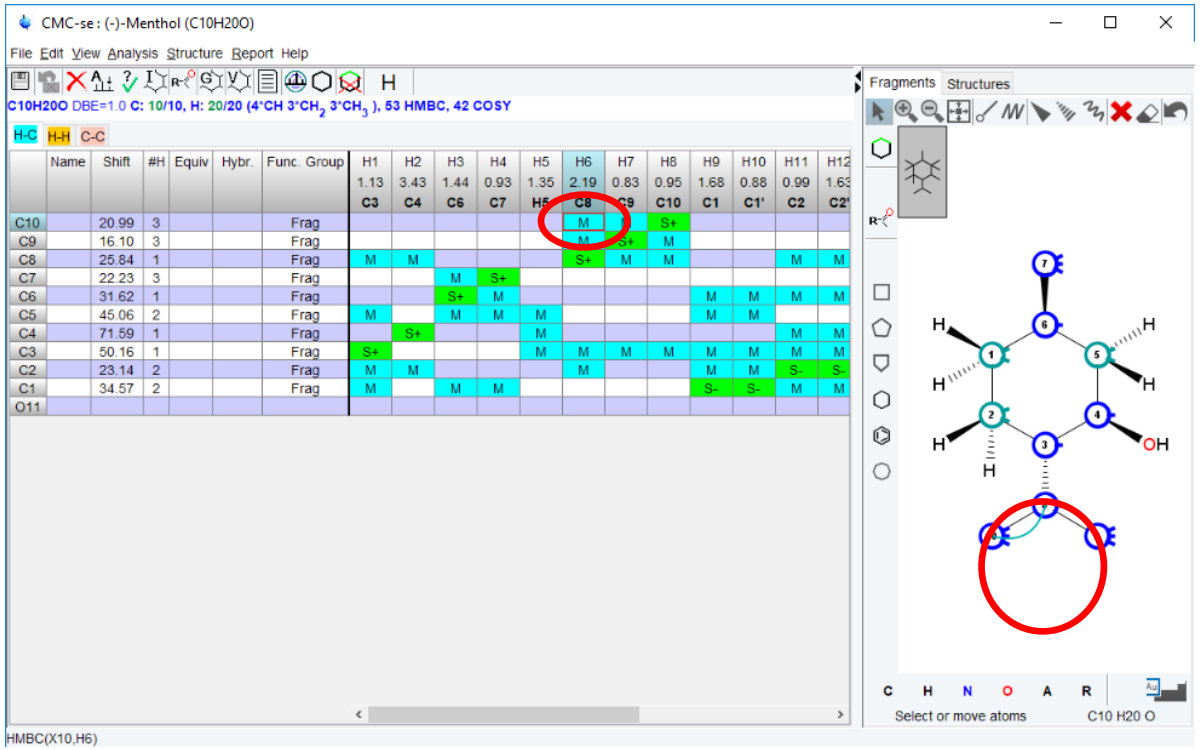
NMReData Import





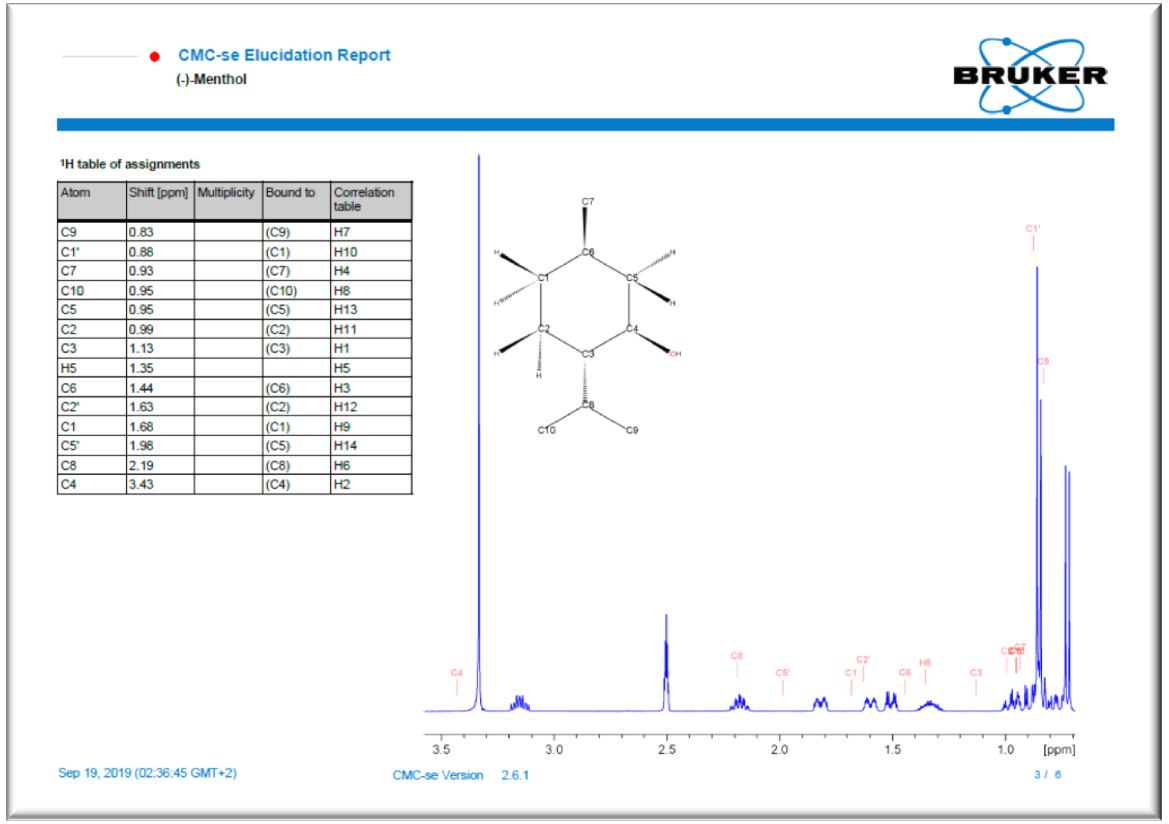
NMReData Import

Detailed data inspection available



NMReData Import

Reporting



CMC-se Elucidation Report
(-)-Menthol

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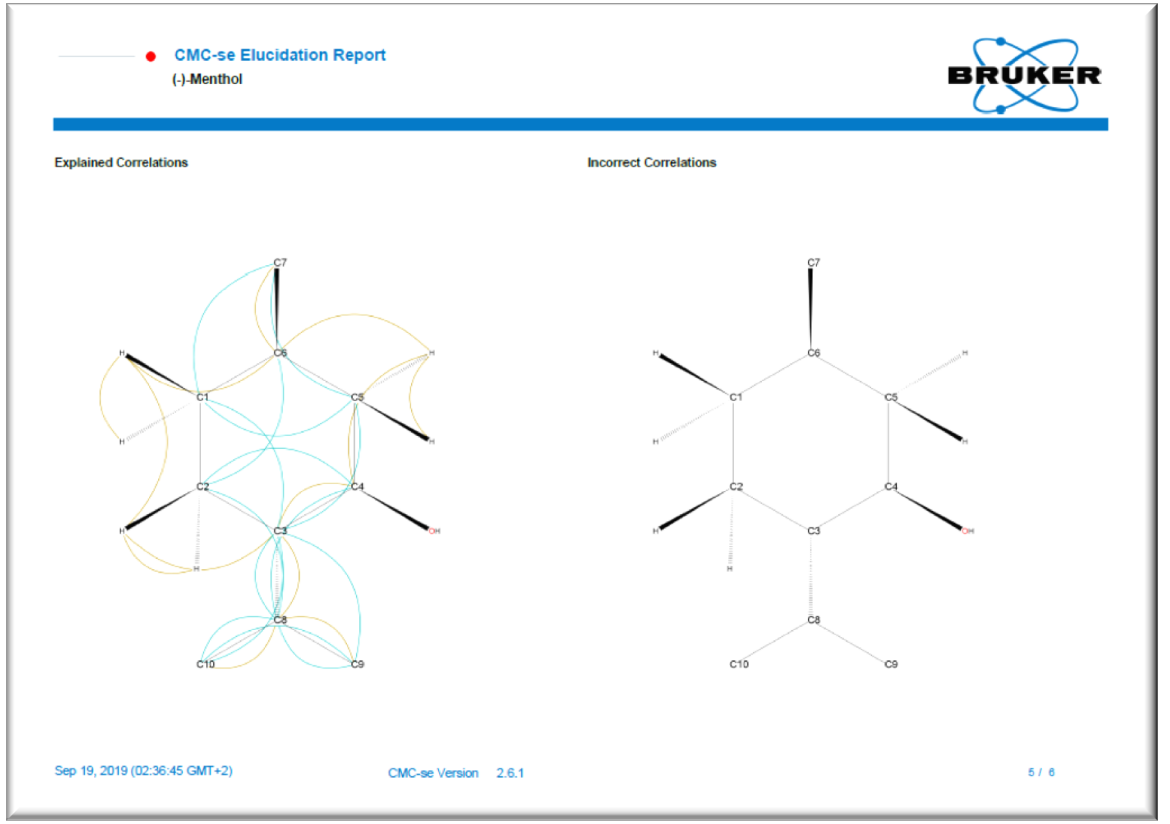
¹H table of assignments

Atom	Shift [ppm]	Multiplicity	Bound to	Correlation table
C9	0.83		(C9)	H7
C1'	0.88		(C1)	H10
C7	0.93		(C7)	H4
C10	0.95		(C10)	H8
C5	0.95		(C5)	H13
C2	0.99		(C2)	H11
C3	1.13		(C3)	H1
H5	1.35			H5
C6	1.44		(C6)	H3
C2'	1.63		(C2)	H12
C1	1.68		(C1)	H9
C5'	1.98		(C5)	H14
C8	2.19		(C8)	H6
C4	3.43		(C4)	H2

Sep 19, 2019 (02:36:45 GMT+2) CMC-se Version 2.6.1 3 / 6



CMC-se Elucidation Report
(-)-Menthol

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Explained Correlations

Incorrect Correlations

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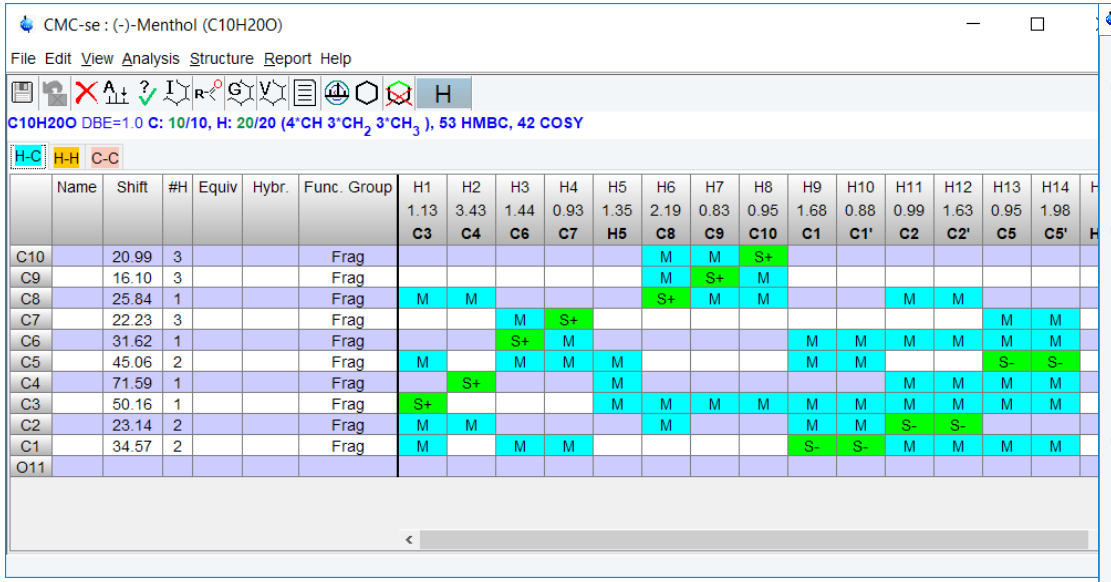
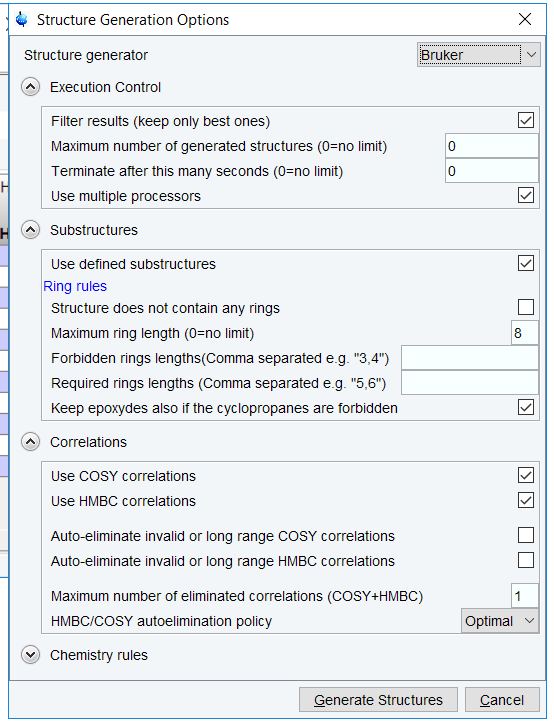
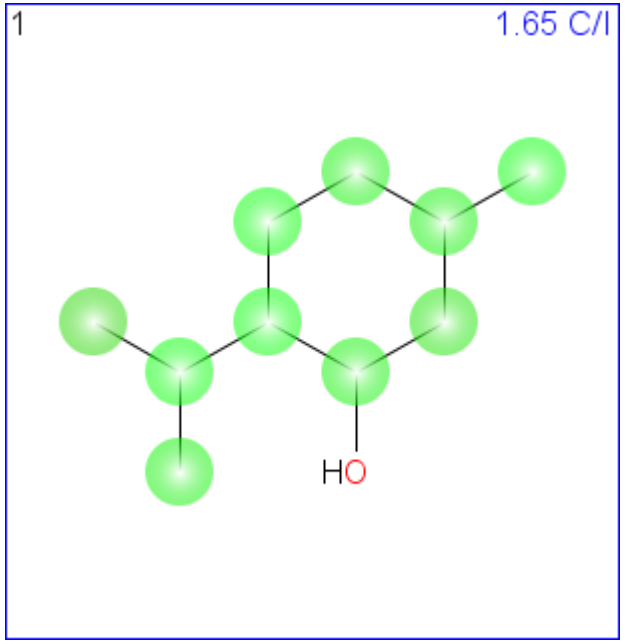
NMReData Import

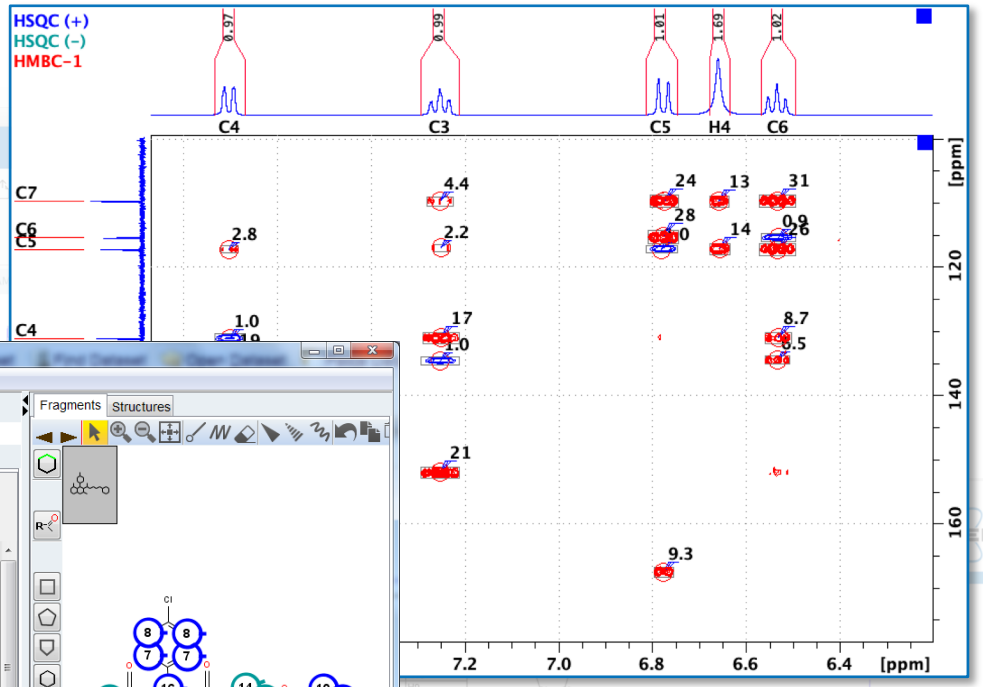
Beyond the data inspection: generate any structure proposals matching the data

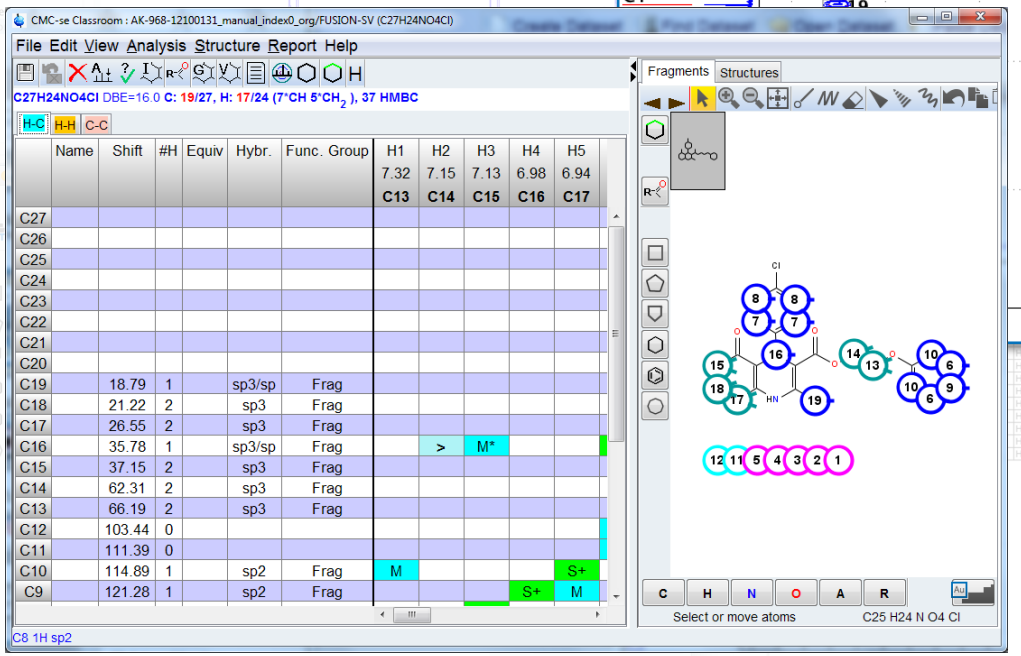






NMReData Implementation Availability





CMC-se

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~~

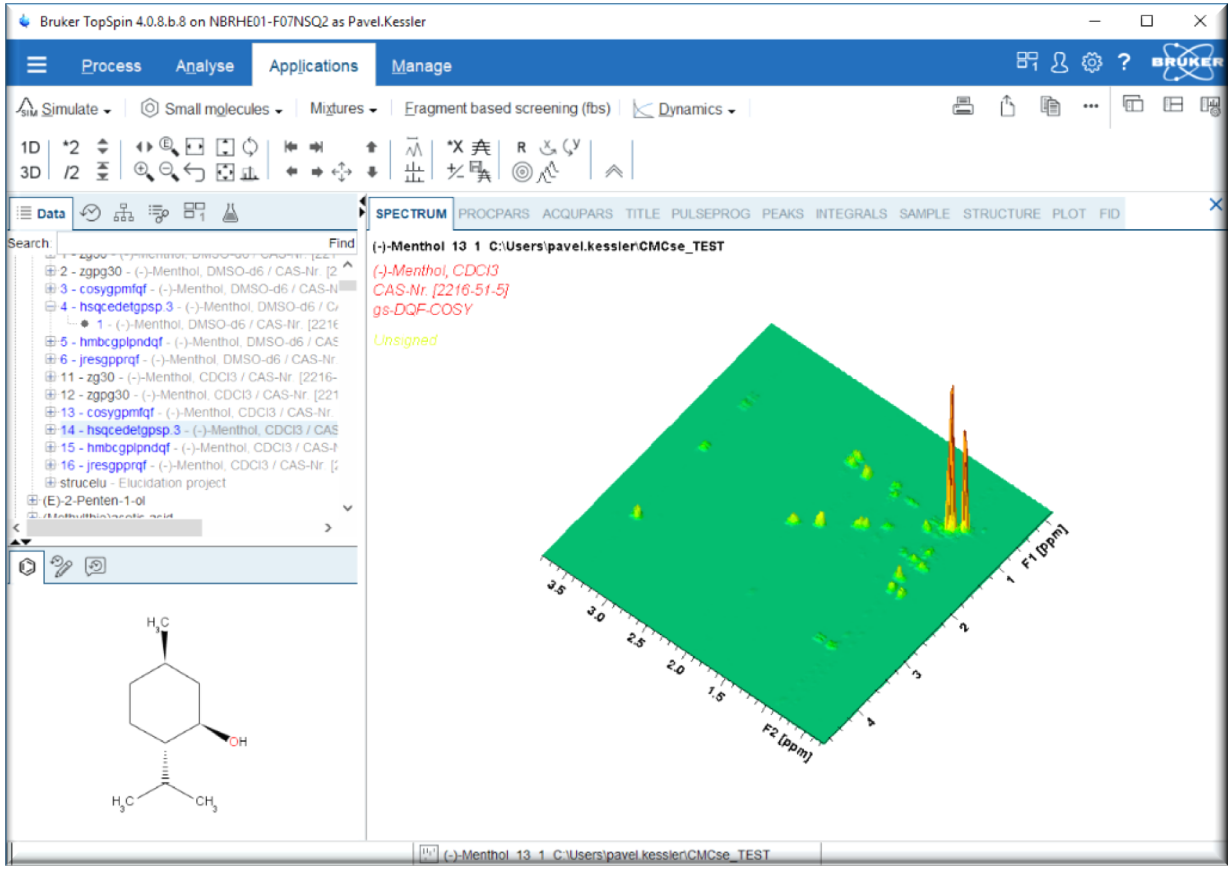
NMReData Implementation Availability

- 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

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> <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!