CMC-se
Assisted Structure Elucidation and Verification

Acquired Data

Structure Verification

Structure Elucidation

Populates Table

Table Refinement

Bruker Structure Elucidation

CMC-se Version: 2.5.1
TopSpin Version: 3.5 pl 6 (of August 4 2016) - Build 1784

Close
CMC-se 2.5
Structure Elucidation/Verification

- **PROTON**
- **HSQC**
- **HMBC** (Required)

- + any additional spectra as
  - C13
  - COSY
  - N15 HSQC/HMBC
  - H2BC, ADEQUATE ... (Optional)
CMC-se 2.5
Assisted Structure Elucidation and Verification

Easy of use

Support for bigger molecules
- Performance improvements
- Simplified fragment handling

Handling of underdetermined structures
- Use on-the-fly ranking

Improved data analysis
- Seamless integration of additional data in existing project

General usage of charged atom states
- Functional groups
- Inner salts

Verification
- Use partial assignment
CMC-se Workflow

![Screenshot of the software interface showing project creation and sample details.](image)

### Project Details
- **Project Name:** strutel
- **Location:** C:\Users\pavel\CMCse\REFERENCE\Pioglitazone_C19H20N2O3S

### Sample
- **Molecular Formula:** C19H20N2O3S
- **Solvent:** DMSO

### Description
- **Options:**
  - Derive proton names from skeleton atom: unchecked

### Used Spectra

<table>
<thead>
<tr>
<th>#</th>
<th>Valid</th>
<th>Description</th>
<th>Solvent</th>
<th>Path</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>✔</td>
<td>PROTON [1H]</td>
<td>DMSO</td>
<td>Pioglitazone_C19H20N2O3S</td>
</tr>
<tr>
<td>2</td>
<td>✔</td>
<td>C13 [13C]</td>
<td>DMSO</td>
<td>Pioglitazone_C19H20N2O3S</td>
</tr>
<tr>
<td>7</td>
<td>✔</td>
<td>COSY [1H, 1H]</td>
<td>DMSO</td>
<td>Pioglitazone_C19H20N2O3S</td>
</tr>
<tr>
<td>3</td>
<td>✔</td>
<td>HSQC [1H, 13C]</td>
<td>DMSO</td>
<td>Pioglitazone_C19H20N2O3S</td>
</tr>
<tr>
<td>5</td>
<td>✔</td>
<td>HMBC [1H, 13C]</td>
<td>DMSO</td>
<td>Pioglitazone_C19H20N2O3S</td>
</tr>
<tr>
<td>6</td>
<td>✔</td>
<td>HMBC [1H, 15N]</td>
<td>DMSO</td>
<td>Pioglitazone_C19H20N2O3S</td>
</tr>
<tr>
<td>4</td>
<td>✔</td>
<td>HSQC [1H, 15N]</td>
<td>DMSO</td>
<td>Pioglitazone_C19H20N2O3S</td>
</tr>
</tbody>
</table>
CMC-se Workflow Analysis
CMC-se Workflow
Interactive data inspection
CMC-se Workflow
Structure Generation

Structure Generation Options

Structure generator
- Execution Control
  - Filler 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
  - Enable substructure filtering
  - 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. "3,5")
    - 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)

- Chemistry rules

Generate Structures | Cancel
CMC-se Workflow
Inspect the results
### CMC-se Workflow

**Additional input**
CMC-se 2.5 News

**Easy of use**
- Generated structures may be edited

**Support for ROESY experiments**
- Interactive definition of relative stereochemistry (Up/Downs)

**Display of correlations reworked**
- Allows to build up the structure manually

**Interface to CSEARCH Robot Referee**
- Structure Assignment Check
- Dereplication
CMC-se 2.5 News
Generated structures may be edited

- Add explicit proton(s)
- “Refine” the structure
CMC-se 2.5 News
Support for ROESY experiments

• ROESY/COSY correlations connect the respective protons

COSY

“Thru space ROESY”
CMC-se 2.5 News
Support for ROESY experiments

- Define the relative stereochemistry
CMC-se 2.5 News
Display of correlations reworked

• Selection of visible correlations
CMC-se 2.5 News
Display of correlations reworked
Valpolicella Superiore Ripasso  
Montere DoP

- Corvina
- Molinara
- Rondinella
- Corvinone
- Rossignola
- Negrara, Barbera, Sangiovese Bigolona

Sensoric analysis

Primitivo !?
PCA of LC-MS data obtained from SPE extracts
Non-targeted time slice-SPE-NMR
Injection: 5x10uL -> 55 SPE extracts in CD$_3$OD
Corvina vs. Primitivo
Aromatic region

Cartridge E4

quercetin
NMR spectra of *corvina* and *primitivo* marker after isolation and cleaning.
Structure elucidation using CMC-se: Corvina

<table>
<thead>
<tr>
<th>Atom</th>
<th>Shift [ppm]</th>
<th>Multiplicity</th>
<th>Bound to</th>
<th>Correlation table</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>6.1</td>
<td>5 (C12)</td>
<td>H5</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>6.24</td>
<td>4 (C15)</td>
<td>H4</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>6.84</td>
<td>2 (C11)</td>
<td>H3</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>7.53</td>
<td>3 (C10)</td>
<td>H2</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>7.54</td>
<td>1 (C6)</td>
<td>H1</td>
<td></td>
</tr>
</tbody>
</table>
Structure elucidation using CMC-se:
Primitivo
Extracted rows from time slice

m/z 477?
CMC-se in the practice
From a Diary of an Oenophile

Unknown substance

C21H18O13

30 HMBC + 3 COSY

29 Unique correlations

(21+18)/29 = 0.74 correlation / atom
CMC-se in the practice
From a Diary of an Oenophile

Unknown substance

1) Try to identify it

http://nmrpredict.orc.univie.ac.at/similarresult/4ab0/4ab05b8101f4069625c548caa0214549_summary.html

***** This URL will be active for 30 days *****

Thanks for using CSEARCH-technology - your feedback is highly appreciated
CMC-se in the practice
From a Diary of an Oenophile

Unknown substance

1) Try to identify it
CMC-se in the practice
From a Diary of an Oenophile
Conclusions

- NMR is the method to detect falsified or wrong declared wines.

- SPE NMR and CMC-se are appropriate tools for the identification and elucidation of components in wines

- **Miquelianin** identified as a marker for Corvina wines
  - It exhibits antioxidant and antidepressant activities
  - It is able to reach the CNS after oral administration

- ✓ *Makes red wine happy?*
Acknowledgments:

Markus Godejohann, Bruker