TopSpin + CMC-se and CMC-assist
last update: 18 Mar 2013 (cgf)

Bruker provides structure elucidation tools in CMC-se, and structure verification tools in CMC-assist. CMC-se requires TopSpin 3.2. CMC-assist is provided independent of TopSpin, but provides a similar (nearly identical) interface, plus the verification tools. CMC-se has some useful features in general for working on combined datasets, defined as a **Project**. Data can be in different expno’s in a single folder, or in different folders.

I. CMC-se:

1. Acquire data following parameter definitions in Bruker’s CMCse_* parameter sets. The higher resolution involved with this data is important. Phase cycles should be NS = 2\(i\) as a minimum, 

   and conservative repetition delays and other parameters related to relaxation (e.g., D8 as mix time in selnogp) are important.

2. Process all data first, minimally with **efp** (1D) or **xfb** (2d – remember to **xf2m** on hmbc datasets; see the pulse program listing for assistance in performing proper processing steps).

   Define multiplets first? 1H and 13C…

3. **ANALYSE → STRUCTURES → Structure Elucidation** or **cmcse**

4. Define the **Project** by adding all data. A **PROTON** and **HSQC** (edited) must be included. The software will also accept: **COSY** **HMBC** and **C13CPD** data as part of a project. The COSY is the least important of the five types.

5. In the table view, click **A** to start the analysis. Look at the pdf report that is generated, especially at the consistency check toward the end.

6. Generate structures using **C**. Scores are based on closeness to 13C δ.

   a) Long-range correlations in COSYs and HMBCs must be eliminated (or allowed to be eliminated; usually enabling 2-4 to be eliminated).

7. Make corrections in the spectra and various tables, guided by the consistency check. # H and # C should equal that in the enter molecular formula.

   a) In spectra, right-click to delete or add multiplets.
   b) In tables, right-click #H to change to match mol formula.
c) In tables, fix 1H multiplicities.

8. Rerun the $\text{\(\text{H}\text{(?)}\)}$ and $\text{\(\text{G}\text{\text{?}}\)}$ analysis.

9. Now rank the structures using $\text{\(\text{F}\text{\text{?}}\)}$ in the table view Structures tab (on righthand side). The scores are listed in the right corner of the structure window: $\leq 5$ is good, $> 5$ means that structure is unlikely to be correct.

10. Use the fragment tool to require and omit various fragments that are already known.