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.

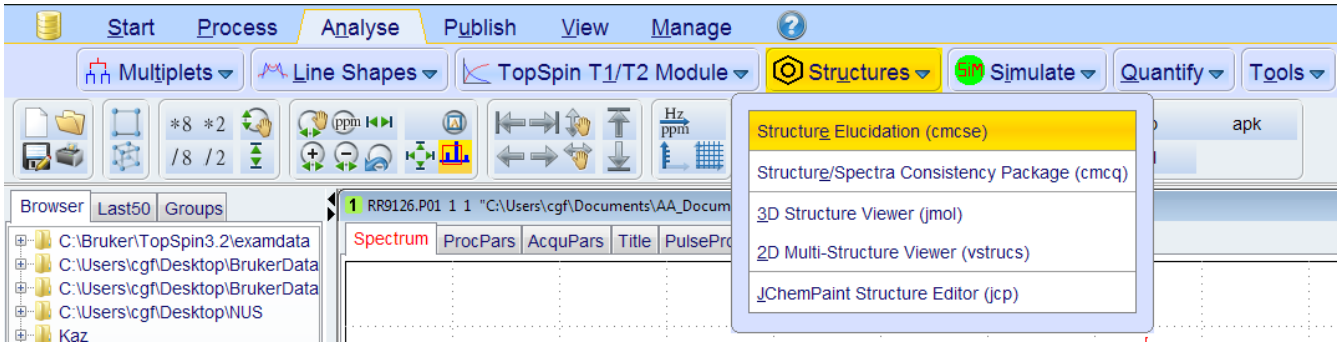
I. CMC-se:

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  to start the analysis. Look at the pdf report that is generated, especially at the consistency check toward the end.

6. Generate structures using  . 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  (?) and  analysis.

9. Now rank the structures using  in the table view Structures tab (on righthand side). The scores are listed in the right corner of the structure window: ≤ 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.