Various, Assignment Aids

Syllabus has been updated

TOCSY review

heteronuc correlation after digression

Databases, knowledge bases for NMR:

    Your noggin should be the primary source material!

      Chem 605 will greatly improve use of that database…

    Reich website

    E. Pretch etal, "Struc Determ of Org Cmds"   [available thru library for download]

    ACD Labs software

    See links on facility website for other on-line resources

MNova

Data analysis and assignments, and publications in MNova

    Settings for Integrations (sum), Peak Picks (GSD), and Multiplet Tool (peaks)

    Sums and peak fitting (example: 3-heptanone):

        baseline correction: can we ignore them?   (YES!   but not always….)
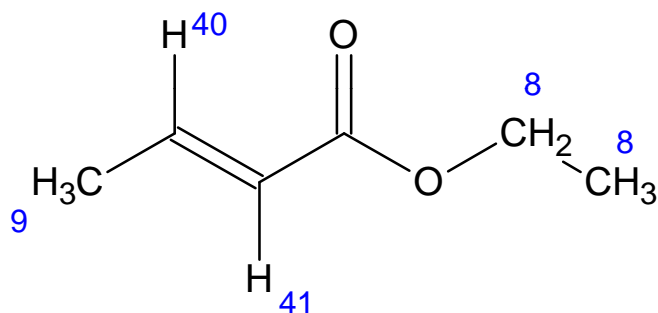
        quantitation of overlapped peaks (peak fitting!)

        correcting multiplet analysis (whoops….)

Automation can be very helpful, but *always* review what it's done (wrong).

11 Nov 2014 – Chem 636

Quantitation: Relaxation!

Preamble to relaxation (next week)

ethyl crotonate: how long can T_1 get?

Ethyl crotonate

T1 (sec)

How would   zg vs zg30   change a ^1H 1D spectrum?