Spartan Tutorial - Modifications for use of the version of Spartan in the CRC

- for both versions, under "Model" you may choose various ways to view the molecule. Wire, or ball and wire, or ball and spoke are probably easiest to interpret.

- if, when you log in, the spartan icon is not present, just go into the destop folder, choose "open unix shell", type in "spartan" and hit enter.

- the minimize button on the Builder window is in the menu bar, not at the bottom.

- "save as" = "save"

- instead of using MM2 as the molecular mechanics routine, use MMFF94. The energies will differ slightly from the energies obtained with MM2, but the difference in energies, which is what is important will not differ by much and the trend, which is most important, will be the same.

- Setting up Calculations: after choosing "Mechanics" (or Semi-empirical), under "Task", select "Conformer Search - Multiple" instead of "Geometry Optimization".

- after the calc has finished, a window showing a list of conformers comes up. Under "Column", select "Energy" and "kcal/mol". This will assign the conformational energy to each conformer. What you are most interested in is the minimum energy of the minimum energy conformer. You may click on the different conformers to see what they look like. For example, check the lowest energy conformer and the highest energy conformer and think about why one might be more stable than another (steric reasons). You can even play with the plot menu to get a plot of energy vs molecule, but this is not necessary for the present task. Note that for the CRC version of Spartan, you may get fewer conformers after doing the conformer search than you would using the orglab version. This is because conformers having identical energies are not repeated in the CRC version. This will not matter since all you really want is the lowest energy conformer.

- to go on to the next molecule or next calc, you need to delete all the conformers and redraw the next (or same) molecule. This is because "Close" doesn't close the conformer window and this is the only way I know of doing it.

- it would be a good idea to compare your numbers with those of someone who did the calc's on the orglab sgi just to be sure everything is working ok. For the two cases I tried, they agree.

- let me know if something is confusing or incorrect or if you figure out a better way to do things.