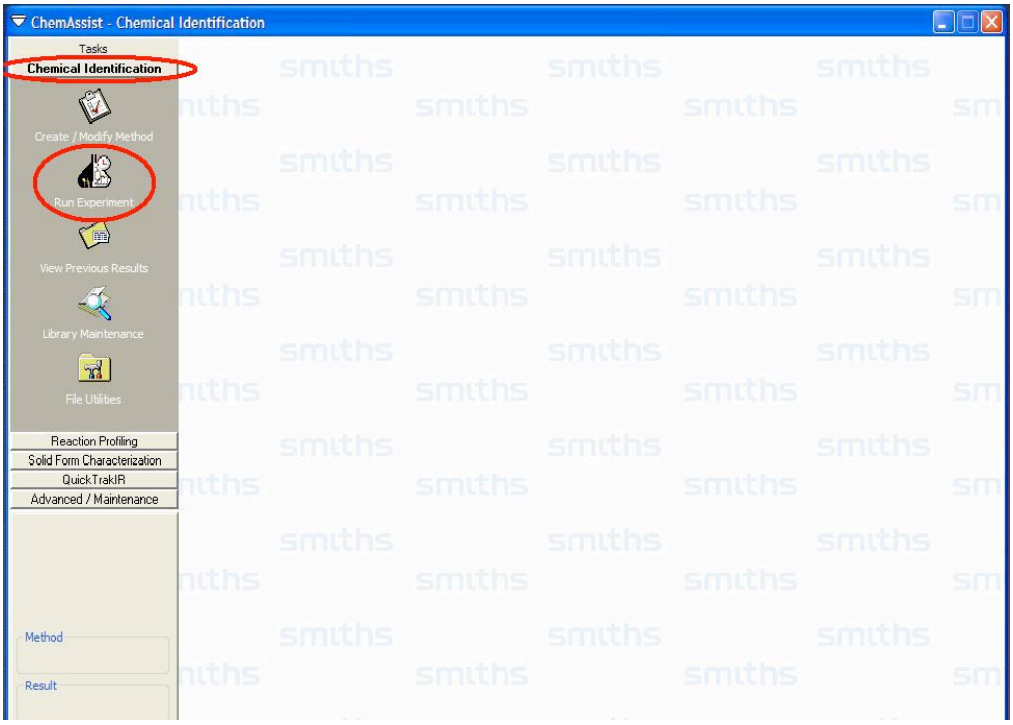
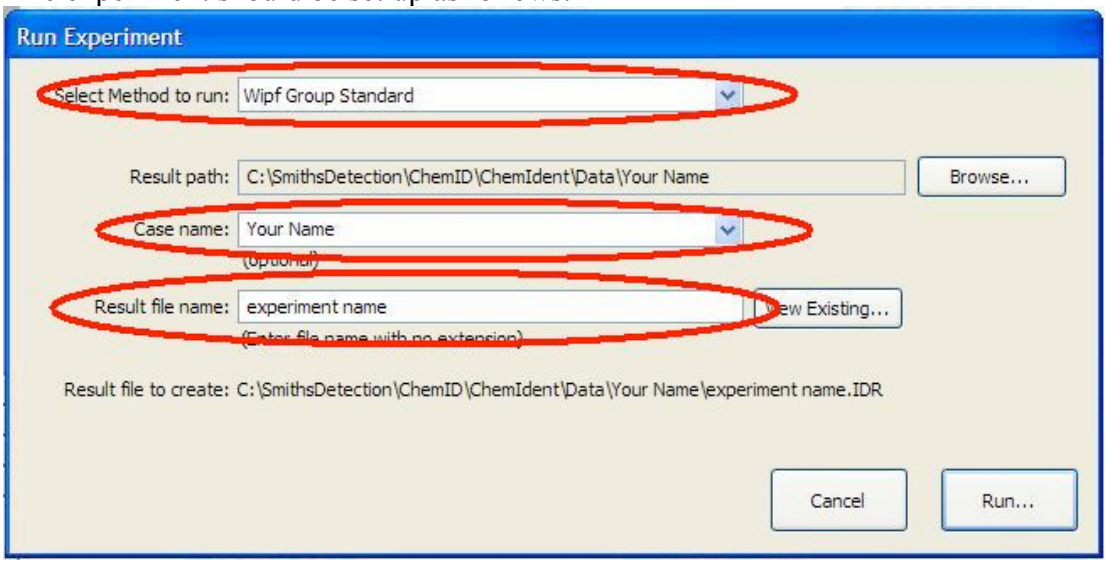
Quick guide for running a simple ATR/IR on the Smith instrument on solids or liquids

Plug in and power up the computer and IR.

1. Log into the computer using the appropriate UID and PW
2. Open the program ChemID, located in the top right corner of the screen.
3. In the window that opens, select "Run Experiment" from the Tasks > Chemical Identification tabs on the left hand side.



4. The experiment should be set up as follows:



The case name will create a folder in the data folder for your spectra that you can access via the shortcut on the desktop. The "Wipf Group Standard" method settings are for a new

background for every sample, resolution of 4.0, number of scans for both background and sample 16. If you need to change this for any reason see Chris R. Select "Run"

5. Select "Acquire Sample"
6. Make sure the sample plate is clean and clear of any debris.
7. Select "Acquire Background" and wait for the background to collect.
8. A) If you are characterizing a solid sample place a small amount (enough to cover the lens on the plate will be plenty) and turn the press clockwise until the pressure gauge, located at the top of the window, reads 60.
   B) If you are going to analyze a liquid, obtain and place the liquid well over the lens and put 1 or 2 drops into the well. (if you are analyzing a significantly volatile liquid place the volatiles cover over the liquid well to prevent evaporation)
9. Select "Acquire Sample"
10. Select "Accept Data" (If you are not pleased with your data select cancel and go back to step 8)
11. Data collection is now complete and remove your sample from the lens. **Using ethanol and Kimwipes (provided) wipe down the sample area, including the plunger, and any solid or liquid that may have spilled.**
12. Select the "Spectrum Analysis" tab
13. By right clicking on the spectrum you can choose to pick peaks manually (Quick peak) or automatically (Auto peak pick). Auto peak pick is the easiest but still requires you to click at the starting and stopping points to define which peaks will be analyzed.
14. Select the "Report" tab. Review your report and make sure that the boxes in the "Report Sections" that say "Spectrum Analysis" and "Peak list" are checked.
15. Select "Print…" and choose "primoPDF" as the printer.
16. PrimoPDF will start automatically and you should change the name from "output.pdf" to your file name. Selecting "OK" will save a PDF copy of your report to the desktop, which will allow easy upload to your CBIS e-notebook from the IR computer. This computer is setup to connect to WipfNet and there is a bookmark to access CBIS. Once you have uploaded your IR report to your e-notebook delete the PDF from the desktop. **NOTE**: Files left on the desktop or folders created on the desktop will be removed weekly without notice.
17. Turn off both the IR and the computer. Unplug and wrap up the cords for the IR and computer and bring the cart back to the small instrument room in 1310.

If there are any questions, comments, or concerns contact Chris Rosenker, 1310, cjr34@pitt.edu