Collecting a FT-IR Spectrum (or trace) using the QATR10 module or sample compartment.

1. Getting Started:
    - HP Workstation – no login credentials req'd.
    - Open **LabSolutions IR**
        - User ID: Admin / Password: _____
    - LabSolutions IR Splash Page
        - Choose **Spectrum** for ABS or %T measurement of prepared samples.
            - Note: spectrum files can only be open in either Spectrum or Postrun, but not both.
        - Choose **Postrun** to manipulate *already saved* spectrums.
2. Spectrum:
    - Find the Instrument ▼ in the scan toolbar
        - **Connect** (if the instrument has already been **Initialize**d, the **Monitor** tile will be green)
            - Instrument Operation area (at far right)
                - Humidity/Lamp/Laser/QATR10 module; all should be green
    - Load Parameters to "blank the system" and avoid what previous users may have done.
        - **CEST_QATR10_Basic** (7800-400 cm^{-1})
            - Data parameters for 95% of users mounting via the diamond ATR.
            - Cutoff set to 4500, but can be extended to 7800 if desired.
            - This choice will default to a CEST folder, to be changed below.
        - **CEST_Sample_Holder-KBR** (7800-350 cm^{-1})
            - Data parameters for sample compartment users (IR cards, pellets, etc).
            - If you're planning this route, you need CEST Staff's help!
                - We need to install the sample holder (cassette), prepare the sample compartment area and securely stow the QATR10 module.
                - *Don't go rogue!*
    - Data tab
        - Alter parameters ***at your own risk***: mode, # of scans, resolution and wavenumber range.
            - Measurement Mode > Interferogram/Power/%Transmittance/Absorbance
            - 8 should be plenty, but alter scan # based on lab protocol, published paper or answered prayers.
            - 4 cm^{-1} resolution *will be sufficient* for almost all users and this already maximizes the S:N ratio.
            - Narrow your range as desired, *but no data will be collected* at 4504 cm^{-1} if you set the limit to 4500 cm^{-1}.
    - Filename click … to open/create a new spectrum file inside a nested User folder within your Lab folder
        - Name as you'd like, but good idea to include initials and date
    - Comment area to describe sample particulars you won't remember 6mo from now (sample was dried for 48h, membrane kept tearing because it hates me, etc.)
        - It seems like Sample Name and Sample ID are kinda useless fields, so just utilize a new filename per sample instead.
    - **BKG Scan** click the tile to make a background scan from the scan toolbar.
        - You will have an opportunity to clean the crystal before proceeding; do so when the warning pops-up.
        - On this unit they are cached or "volatile" and do not save as a separate file, unlike your spectra.
            - You should run a new background everyday, or
                - if you are switching among measurement modes
                - between time gaps among samples (ran in the AM, went to lunch and are running now in the PM).
    - Leave the **View** window and return to the **Measurement** window
    - **Sample Scan** click the tile to analyze a sample from the scan toolbar.
        - *There is no warning, it will immediately scan whatever is (or isn't) mounted on the crystal.*
            - A scan counter will show up (briefly!) in the bottom left of the screen.
        - You will be automatically taken to the **View** window to see your completed spectrum.
        - Each collected spectrum will hang out in the file browser tree (at upper left) in order of analysis.
3. View (= Postrun):
    - Things you can do in here include:
        - Print preview a report about your spectrum; we've narrowed this to a "simpler" report choice for most users.
            - We'll use *Data_p_1page* to demonstrate.
        - **Search** / **Edit Library**

- Choose some or all of the Libraries (14+ classes) from the General tab (at right) then click
- **Spectrum Search**
  - Choose from 12,000+ spectra; but we plan to get more ATR-specific libraries.
  - Ranked by highest score; a 999 score is the absolute best match for your spectra and a library item.
  - **Join** the spectra to overlay the target spectrum with the top choice from the hit list.
  - **Difference Factor** will calculate the deviance between both spectrums, if you click **Done** it will save this to your spectrum (*BE CERTAIN YOU WANT THIS TO BE DONE!*)
- **Edit Library**
  - Add a spectrum you want saved into the library database from the file browser tree, right-click on filename, **Insert into Library** and **Yes.**
    - Maybe you will be working with a compound regularly that is endemic to your samples and you want to add it into the library for subtraction purposes; great that is why this option exists!

- Manipulation
  - **Peak Pick**
    - You can move to Postrun from within Spectrum, see bottom left "**Move to Peak Pick Screen ▼**."
    - Automatic peak picking after clicking **Calc** is threshold based, so minimally absorbed or transmissioned (I made that up, lol) peaks may not get labeled.
    - Manual peak picking is your best choice, use mouse clicks to zoom-in and place a rectangle over a peak: **Add peak** and doubleclick to zoom out; this will take some practice.
    - If peaks labels are saved, they appear to not be removable from the saved file *later*; perhaps save as an altered file, like *MySampleIsSpecial_peaks* or something like that.
  - **Data Calculation** = Difference Spectrum
    - Subtract a reference spectrum from a target spectrum; **Calc** will process the spectrum and **OK** will save a result.
  - Other relevant Data Processing options:
    - **Normalize/Baseline Correction/Smoothing/ATR Correction/Atmosphere Correction**
      - These are all pretty self-explanatory, but we can consult the Shimadzu manuals for more detail. **Calc** will apply, **Cancel** will not save any changes.
  - File menu > **Window**
    - **Join All** vs. **Split All;** typically View will show each loaded spectrum as its own tab.
- Data Export
  - I will flesh this area out later, but use CSV .txt files, probably the most universal option.
  - No sign yet that LabSolutions IR can read older Bruker files, but maybe try loading an old .dpt export and see?

4. Wrapping up:
   - Close LabSolutions IR (no need to unload samples).
   - Clean up work area, make sure usage details are recorded in the shiny new logbook.
5. ATR module details that should be covered in-person:
   - Clamp Anvil Arm Assembly
     - **Self-levelling flat tip**: *use this for solids, films and powders.*
     - **Concave pellet tip**: *use this for polymer beads or softish irregular shaped solids.*
     - Liquids: *no tip necessary, confidently "park" the anvil to the left or the right - your choice!*
       - **Volatiles cover**: *use this with liquids that are not liable to hang around too long; you know the ones.*
     - **Torque Limiter Screw Knob Assembly**
       - The knob on-top will tighten down clockwise until the load is set; you will feel the slipping difference (and hear a "click") when you continue to rotate the knob at this point.
         - Great! Now we're applying the required 40lbs of pressure over the anvil face.
   - Our diamond crystal is in the middle of the silver puck; it is a very smol area.
     - Don't break it.
     - Clean with 95% ethanol, methanol, acetone or water.
     - Clean off any residual moisture before leaving the area.