## 4. GETTING STARTED

This video begins the demonstration lesson, also described on-line in our Training Guide as "lesson 1." I'll be following what's written in our basic instructions line-by-line, so I recommend having a copy nearby. The instructions are on our website (nmrlab.technion.ac.il) under Instructions, DPX200, <sup>1</sup>H NMR, 1D acquisition and processing.

The instructions generally include two options – one for the keyboard and one for the mouse. On-line you'll find hyper-links with further details. You can find copies of the software manuals in the lab and you the help menu of the program is handy. However, the instructions we will follow are sufficient for now.

Let's start with step 1(a) of the instructions. Sign the logbook with your name and phone number. Topspin should be open, if not, just click on this icon to open the program.

Step two now, is to create a new file. Let's click here on new. "Name" is the name of the file. I'll add 200 to my name to keep me organized, since I'm sitting at the 200. The experiment number should be an integer number, no letters and no symbols. The process number should be 1. The data directory is on /opt/topspin, so keep that as it is. Our convention is to type your advisor's name where it says user. First Initial, no punctuation, then last name. This is, again, to keep the files organized.

A note of warning, as a facility manager, I reserve the right to delete files on this computer at any time, So, BACK UP your data. I'll explain a number of backup options after we've acquired our data.

Continuing with the creation of a new file, here I select the solvent. Here I choose a standard proton NMR parameter set. On the keyboard, type 1H. Wth the mouse, 0\_1H is exactly the same parameter set, it's just at the top. Here I type a title. And now I click, "ok." That's it.

Across the top of the window here is all the information we just entered. If I click on acquisition parameters, I see that the experiment I chose has already provided me with some starting values for acquiring a <sup>1</sup>H NMR spectrum. Later I will want to optimize these to my particular sample, but these values are a good place to start.

As an aside, I highly recommend opening a text document or spreadsheet and maintaining a list of experiment numbers and titles. It only takes seconds if you create it as you go. If you wait until you've acquired a couple hundred spectra, it takes much longer to reconstruct such a list. Here I'll put in date, experiment number, and title. I could add more details. Later you can store it as an index with your data; it's very easy this way to search for an unknown experiment number by date or by title.

While we're navigating files outside of the program Topspin, you can see here what happened in step 2: /opt/topspin/data/user/nmr/name/experiment# and the various files. There isn't yet a file called "FID" - that is what we're going to record by NMR.

In the next two videos we'll see how to properly place an NMR sample inside the magnet and then how to prepare the magnetic field for optimum resolution and sensitivity.