Department of Chemistry
NMR Facilities
Director: Dr. Carlos A. Steren

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∗ To check on the **instrumental status** and **reservation system**, and find tutorials, links and more, visit our website www.chem.utk.edu/nmr

∗Varian 500 MHz. The brand new liquid state NMR spectrometer is located in the SERF NMR Lab. It is in full operation since July of this year. The probe installed is called OneNMR. It is a dual channel multinuclear probe, covering the range from ^{15}N to ^{31}P on one channel and ^{19}F and ^{1}H on the other channel.

A nice feature of the new instrument is the Autotune system. The probe is tuned to the desire nucleus with a click of the mouse.

There are standard experiments set for ^{13}C, ^{31}P, ^{19}F and ^{1}H. If another nucleus is needed, it certainly can be set up.

∗ Comparing sensitivity among our NMR spectrometers: Besides an increase in resolution, a higher field (higher frequency) instrument, means higher sensitivity. A standard sample of 0.1% ethyl benzene in $CDCl_3$ is used to measure the

^{1}H signal to noise. The ^{1}H sensitivity was measured for all the liquid state instruments. The results are detailed below.

^{1}H sensitivity

AC250	V300	B400 (BBI)	V500	V600 (cold probe)
30:1	98:1	234:1	660:1	4356:1

∗ **Chemical shift predictor: NMRPredict** is a routine, part of MestreNova, that predicts chemical shift values. It can predict ^{1}H, ^{13}C, ^{15}N, ^{17}O, ^{19}F, ^{29}Si and ^{31}P spectra. It is very simple to use;

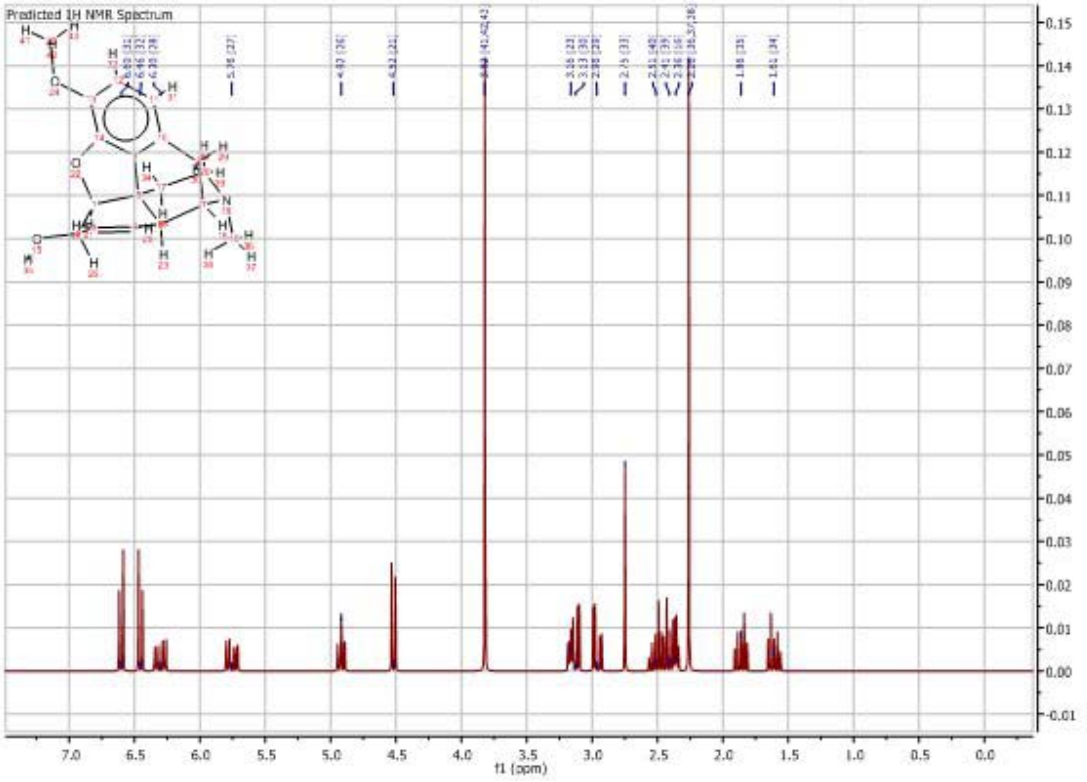
1) Within MestreNova, click on the "Open" icon and open a file containing the molecular structure. It must be in "mol" format. ChemDraw format is not accepted.

2) Click on the tab "Molecule" and select the nucleus that you want to predict. The predicted spectrum will show up.

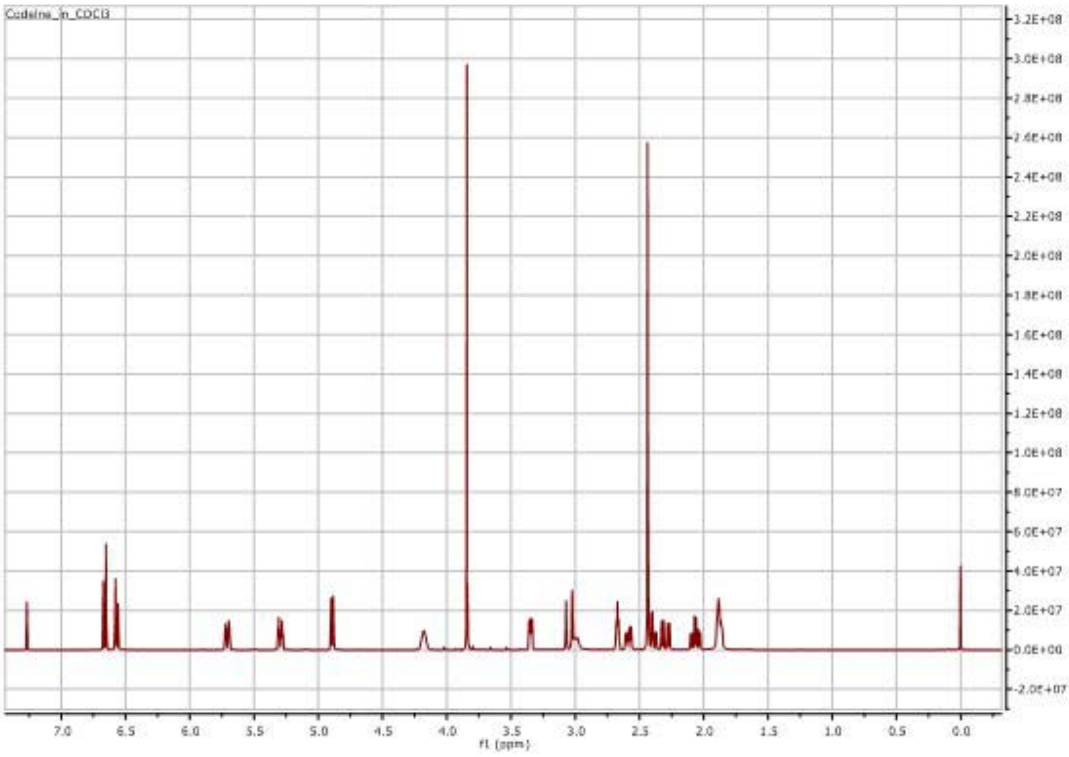
3) The program can also be used to identify cross peaks in an HSQC spectrum.

In the following two pages, I have added the ^{1}H and ^{13}C spectra predicted by MestreNova and the experimental NMR spectra for the compound codeine. Predictions are not perfect, but still, they give an idea of the position of the signals.

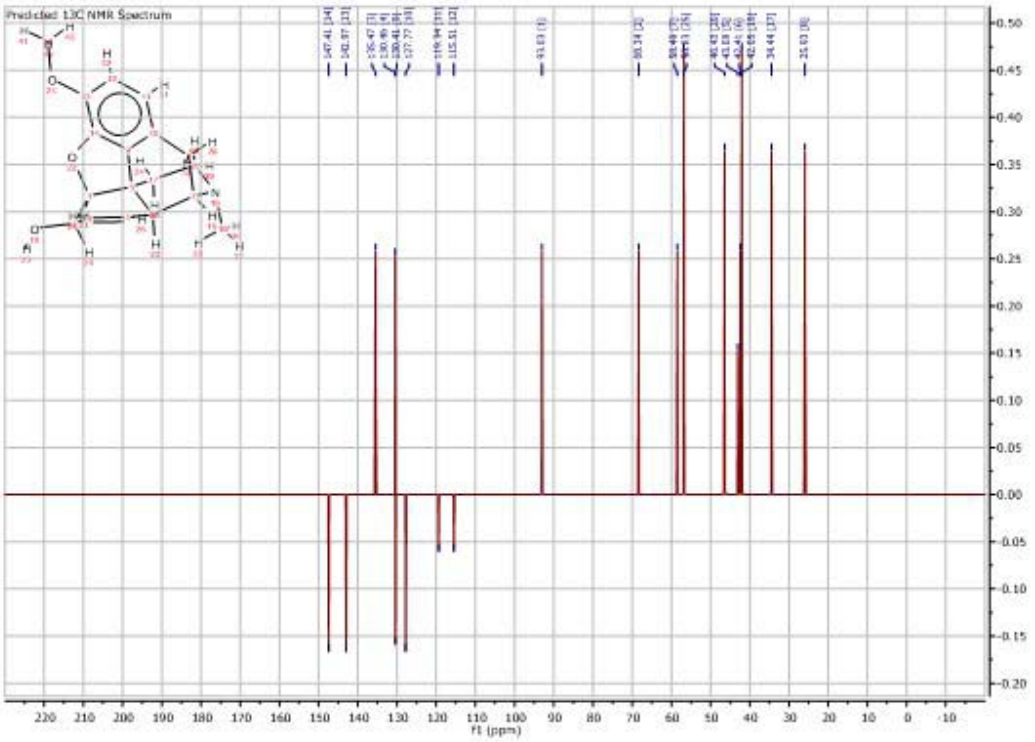
Predicted ^{1}H spectrum of Codeine



^{1}H spectrum of Codeine



Predicted ^{13}C spectrum of Codeine



^{13}C spectrum of Codeine