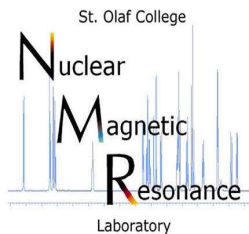


Web-Based Interface Allowing 24-Hour Undergraduate Access to a 400-MHz NMR Spectrometer

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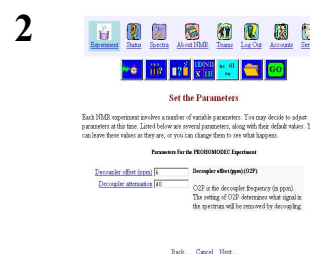
In October of 2002 St. Olaf College installed a fully automated Bruker Avance 400 MHz NMR spectrometer. A project was initiated with the goal of designing, creating, and implementing a web-based, dynamic NMR that could be operated 24 hours a day 7 days a week. Our “24/7 Dynamic NMR” system is now fully operational. Using this system, students, faculty, and guests can select experiments, set parameters, submit IconNMR experiments, monitor spectrometer status, adjust integration and scales, and print spectra from anywhere on campus.



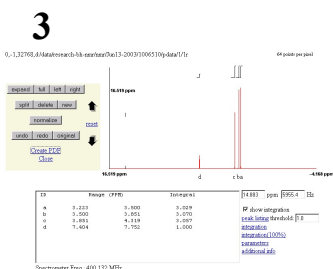
Jared (above)
and Bryan (right)



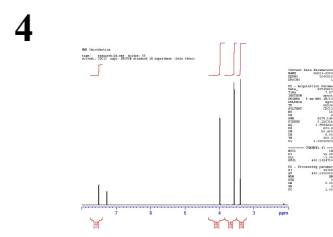
The basic information that is needed for the submission of an NMR experiment remotely includes designating sample position, solvent, experiment, title, and priority. The priorities that can be set include high, normal, low, night, “wait until a certain time,” and hold.



The parameters are experiment-specific. For example, if the user is running a normal proton experiment they will only need to set the number of scans. However, if the user is running a proton homodecoupling experiment, they will need to set the decoupler frequency and power. This is achieved through parameter sets. An explanation of each parameter – what it is, what it does, and suggestions for its use – is given in the space to the right of the parameter list. Default values are provided so that the parameter screen can be skipped if the user is a novice or has no need to set parameters.



Modified “thumbnail” JCAMP-DX data compression is used to deliver the spectrum to the user’s browser, where Javascript functions turn it into an interactive display. Integrals and scales can be adjusted. (We have found no need for routine adjustment of phasing; if this is needed, the user must download the full FID and parameters and use an auxiliary program.)

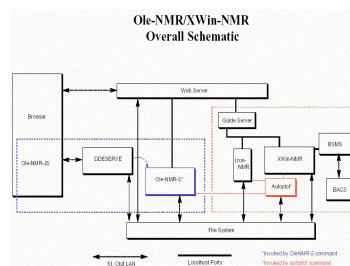


In the end, the spectrum is delivered as a high-resolution color PDF file created by Bruker’s *autoplot* program using a template that separates the spectrum from the integration in a manner that is easily interpreted by undergraduate students.

Further experimentation is encouraged.

How does it work?

“OleNMR” is a combination of client-based Javascript, server-based executable (OleNMR-S.EXE), and selective “overlay” modifications to few files in the Bruker IconNMR TCL library. When the user clicks the submit button, OleNMR-S checks to make sure the user is who they say they are and is only doing what they are allowed to do. An IconNMR “remote processing” file is created, initiating a standard IconNMR experiment. The experiment is scheduled to run based on a novel set of rules we call a “fair queue.”



OleNMR works on all current versions of Netscape Navigator and Internet Explorer. Students in the organic lab are divided into teams, and each team is assigned a sample position on the BACS-120 carousel for the entire semester. Student teams are given free rein to run almost any sample they want. OleNMR is so easy to use a student can run many experiments with just a short introduction. Thus, students in the organic lab no longer have to rely on a lab assistant to run their NMR experiments for them, and NMR can be introduced in an independent “research mode” exactly along the lines of actual research use. Preliminary results indicate that one of the favorite times to submit an experiment is between 10 pm and midnight.

What lies ahead?

We are experimenting with different servers and extending the capabilities of OleNMR, but principally all of the major obstacles have been overcome. As it stands, OleNMR is *the* way students both in courses and in research access the instrument on a routine basis.