NMR Spectroscopy: Learned and Delivered on the Internet

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Abstract: The NMR Collaborative Training Partnership is an NSF sponsored project that provides several nearby two-year and four-year institutions access to a 300-MHz FT-NMR. Using Web-based materials we teach students who do not have direct access to an instrument the basics of how an NMR spectrum is generated. We also have a Web server and remote software that allows students to generate real spectra from samples they have submitted to their instructor. In this way, students who do not have a local FT-NMR can gain experience with this important technique.

[*]Introduction

A medium-field Fourier-transform nuclear magnetic resonance spectrometer (FT-NMR) has been in place at Rider University since 1987 and has played an important role in the training of our students in both the undergraduate and research laboratories. In an attempt to assist two-year college graduates in a seamless transition to a four-year program in the chemical sciences, we are developing a program, the NMR Collaborative Training Partnership (NMR-CTP), which allows students from remote institutions access to a new 300-MHz Bruker Avance FT-NMR installed at Rider University utilizing the internet for data delivery and instruction.

It is well recognized that undergraduate students need exposure to NMR spectroscopic techniques at some point in their college training. Typically, a student's first experience with NMR occurs in the organic chemistry course and laboratory, and it is reinforced in upper level courses. At many undergraduate institutions, the utility of an NMR instrument both in the curriculum and in research activity helps to justify the purchase and maintenance expense of at least a 60-MHz NMR. At the typical two-year community colleges, however, the costs of such an instrument often outweigh the limited use it might get. At Rider University, we have found that the number of students who transfer into our programs from local two-year institutions is on the increase, but, when they come to Rider as juniors, they are not as well prepared to work in the upper-level laboratories as students who have completed their first two years at Rider because they have had little or no access to NMR instrumentation. In response to this need we are developing the NMR-CTP.

Two-year college students in classes that participate in the NMR-CTP prepare NMR samples in their own laboratory during their regular laboratory periods. These samples are then transported by their instructor to Rider and analyzed on our spectrometer. The NMR software has been set up to allow open access to the instrument for multiple users. An autosampler is also installed, which allows large numbers of samples from a teaching laboratory to be run overnight. In some cases the instructor will also bring his or her students to the NMR facility for one visit to observe the instrument working and to observe how an NMR experiment is performed; however, the key to making this program work is access to data. We have set up a computer script, which, on a daily basis, compresses each student's NMR data structure and places the compressed version on a Web server. The next day students can download their data at any remote location with Internet access, so the analysis can be done in a computer laboratory at their institution or even in their own homes. Once downloaded, the data is uncompressed using standard software. Analysis of the NMR data is accomplished using AcornNMR's NUTS program, for which we have obtained a site license. In this way, students have direct access to data from their own samples, and they gain valuable exposure to NMR experiments, sample preparation, and data analysis at the same academic level as their counterparts in a four-year college.

Data acquisition and analysis are, however, only half of the CTP program. We have also developed a Web-based tutorial that takes a different approach than most of the NMR sites currently available on the Internet. Our first consideration is that we have users at many different levels in our CTP. Many of the students participating in this program, including our own from Rider, are still neophytes to NMR and even to organic chemistry. We also have some instructors who have had limited or no experience with FT-NMR. Additionally, some of the users are from nearby four-year schools which have 60-MHz NMR capability, but which use our NMR for higher resolution experiments. To address these concerns, we have targeted our NMR site on the practicalities of obtaining an NMR spectrum, and the material is written with multiple layers. The top layer allows users to navigate through the acquisition of an NMR spectrum in a linear fashion starting from a compound in hand and ending with a spectrum. At every step along the way, however, users can find a deeper level of information if they need help with a particular topic. Furthermore, there is a large clickable NMR glossary to help the students with unfamiliar terms. In addition, there is also a section of the tutorial devoted specifically to how to use the NUTS software. The tutorial itself, while designed specifically for use by the students in our CTP has been developed with outside users in mind as well.

In the year since we installed the Internet-capable instrument, we have been quite successful in developing the capabilities of the instrument and the utilization of the Internet

[*] Presented at the ACS Division of Chemical Education sponsored symposium on web-assisted learning in chemistry at its 221st national meeting in San Diego, CA April 1–5, 2001.

Table 1. List of Participating Institutions

Two-Year Colleges
Bucks County Community College (Newtown, PA)
Mercer County Community College (West Windsor, NJ)
Middlesex County College (Edison, NJ)
Raritan Valley Community College (North Branch, NJ)
Four-Year Colleges
Delaware Valley College (Doylestown, PA)
Monmouth University (West Long Branch, NJ)
Rider University (Lawrenceville, NJ)

connection by the participating institutions listed in Table 1. These institutions have all accessed the NMR-CTP at various levels. It should be stressed that the most critical part of the CTP is the ability for all students to access their own NMR data across the World Wide Web, allowing decentralized data dissemination. This aspect has also been the most tricky to develop, because there are very few models from which to draw ideas for its development. Furthermore, we found that the large volume of data files that were generated took up a large portion of the university's Web server even with the data compression. To reduce the burden to university-wide computing, a separate Web server dedicated to handling the data files generated by student NMR samples, was required.

More information about the NMR-CTP and the online tutorial can be found at http://www.rider.edu/nmr.

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