Remote MALDI-MS Experiments from the Classroom

Ioan Marginean¹, Akos Vertes*¹, Frederick J. Cox², and Murray V. Johnston²

¹ The George Washington University, Washington, DC
² University of Delaware, Newark, DE

Introduction

With the increasing sophistication of analytical tools the traditional classroom experiments in chemical analysis are rapidly becoming extinct. While the complexity of these new tools (e.g., mass spectrometers, gas chromatographs) requires the power of demonstration, their size, weight and the need for various utilities make them laboratory-bound. Thus, there is incentive for bringing the operation and imagery of real instruments into the classroom utilizing remote access via the Internet.

There are several chemistry courses that can directly benefit from remote experiments. For example, at The George Washington University (GWU) Introductory Quantitative Analysis and Instrumental Analysis at the undergraduate level and Spectrochemical Analysis, Ions Wet and Dry and Mass Spectrometry in Life Sciences at the graduate level are amenable for testbed experiments.

It is expected that remote operation of complex instrumentation becomes common in the future. The present entry points of this technology are in the area of experimentation and data collection in hostile environments (space exploration, polar research, battlefield analysis, etc.) and in case of unique and/or major research facilities (e.g., synchrotrons, radiotelescopes). Increasingly complete computer control of analytical instruments and abundant availability of broadband network access enables widespread utilization of remote operation, data acquisition and analysis. Thus, the exposure of students to this technology is highly desirable.

Instrumentation

A time-of-flight (TOF) matrix-assisted laser desorption ionization mass spectrometer (MALDI-MS) – (Biflex III, Bruker Daltonics, Billerica, MA), located at the University of Delaware (UD) was configured to operate over the Internet (1). The control and analysis software was a collection of tightly coupled X Windows applications supplied by the instrument's vendor and ran on the attached Sun ULTRA-5 workstation. The test of remote instrument control was performed on various platforms, including Sun (Solaris), SGI (IRIX), and PC (MS Windows) workstations. The highly automated nature of this instrument provided an excellent opportunity to explore the utility of remote experimentation in a classroom setting.

Both the GWU and UD are Charter Members of the Internet2 initiative, thus, sufficient bandwidth is available for remote control in real time. In the multi-platform environment of instrument control and remote operator workstations, we utilized the Virtual Network Computing (VNC, AT&T Research
Laboratory, Murray Hill, NJ) software package to remotely control all the instrumental parameters and sample manipulation. The VNC protocol was based on the concept of remote framebuffer. The VNC server was implemented on the instrument control computer and the VNC client was running on one or on multiple classroom computers. To aid in sample selection and navigation, an additional streaming video link was established based on a second VNC server and a corresponding viewer. This arrangement provided a complete virtual environment for the remote operator (Figure 1). The graphical user interface of the remote machine showed the complete instrument control panel and the video camera image of the sample surface.

Results and Discussion
In standard MALDI-MS experiments all the important instrumental parameters are computer controlled. A workstation in the classroom served as the instrument interface for the instructor. After loading the samples at the instrument site, the remote operator took charge, monitored the condition of the instrument, selected the experimental conditions, and acquired the data.

Live demonstration of MS experiments and, potentially, hands-on student experience with sophisticated instrumentation, are enabled by the wide availability of computer networks and remote control software. The MALDI-MS instrument, located at UD, was controlled over the Internet from various classrooms at GWU. The Internet-based remote operation of the MALDI-MS system was incorporated into a graduate level course (Ions Wet and Dry), into a presentation on proteomics at the GWU Medical School as well as into presentations on advanced teaching technologies at GWU. The latter also featured remote experimentation from a laptop computer utilizing wireless networking, a very attractive approach for student participation. Different aspects of the MALDI-MS experiment (monitoring instrumental parameters, selecting experimental conditions and acquiring data) were presented to the students. As an example, peptide analysis with MALDI-MS was performed. The 384-well sample holder was prepared with samples of interest and preloaded into the instrument. Several aspects of taking successful MALDI spectra were demonstrated. The effect of laser intensity and the presence of a laser irradiance threshold were shown by systematically changing the laser intensity. The students discovered the existence of sweet spots on the MALDI sample. The impact of selecting the right matrix was established by taking spectra of the same analyte from different matrices. Procedures for linear and reflector mode operation were established. Optimization of some instrumental parameters, such as accelerating, focusing and reflector voltages was carried out from the classroom. Finally, the application of on-line bioinformatics databases in conjunction with remote experimentation was explored.

Conclusions
We have developed an effective method to remotely operate a state-of-the-art MS. Advantages of this approach include hands-on student experience with sophisticated instrumentation from the classroom and better utilization of the available analytical instruments. The utilized systems can be located in smaller rooms that normally cannot accommodate entire classes. Conducting real experiments, as opposed to working with software models, is a more realistic, richer experience for the students. Clearly, simulations are based on idealized situations, whereas using remote instrumentation the students may encounter real problem situations (for example contaminated samples or inadequately tuned instruments). Many students take the lectures without the corresponding laboratory course, thus, depriving themselves of full immersion. These students acquire a more complete appreciation of the presented analytical tools. Finally, improved safety can also be mentioned as an additional benefit. Some of the modern analytical instrumentation present potential safety hazards (high voltage, radioactivity, etc.) even under ideal circumstances. Removing the operator from the vicinity of the instrument minimizes these risks. Currently, the only substantial limitation to remote experimentation is the need for human intervention at sample introduction. The rapid spread of robotics for sample preparation (see, for example, the latest MALDI-MS systems designed for proteomics) will dramatically enhance the capabilities of remotely controlled mass spectrometers and expand their applications beyond the classroom.

Reference