



## A virtual lab for 'mass spec'

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By Byron Spice, Post-Gazette Science Editor

Most people might not know what a mass spectrometer is, but they undoubtedly experienced what these analytical devices can do.

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### Online graphic

[How does a mass spectrometer work?](#)

(.pdf format)

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When investigators on television's CSI: Crime Scene Investigation identify a mysterious chemical, they use "mass spec." Olympics officials use mass spec to check an athlete's urine for illegal steroids. Mass spec can analyze human hairs to detect cocaine use.

Environmentalists use mass spec to study mercury in fish. Mass spec is a major tool used in proteomics, the hot new field of protein sequencing and analysis. And the number of applications keeps growing.

Sometimes it seems the only people not using mass spectrometers are college students.

Ranging in price from \$50,000 to \$700,000, mass spectrometers are too expensive for many smaller institutions and, even when they are available, are often monopolized by faculty members doing research.

So students majoring in chemistry and biology often don't get much training on a tool that they probably will be using extensively in their chosen field.

That circumstance may be changing, thanks to a new system developed under the guidance of two Pittsburgh chemists -- Mark Bier of Carnegie Mellon University and Joseph Grabowski of the University of Pittsburgh -- and presented this weekend by Bier at the American Chemical Society meeting in New Orleans.

Called the Virtual Mass Spectrometry Laboratory, the Web-based system allows anybody to become familiar with running experiments on several types of mass spec. The virtual lab's Web site, <http://mass-spec.chem.cmu.edu/VMSL>, includes several case studies that users can solve using mass spec.

Mass spectrometry is a method of identifying elements and compounds by determining the mass of each atom or molecule. The basic technique has been in use for more than 60 years, though a number of innovations have expanded its uses in the past 20 years, particularly in biology.

Users of the virtual lab must select the correct type of mass spectrometer for the information they need to solve each case study, must choose how to prepare samples and must decide how to adjust the machine's settings.

When users run their experiment, they receive real data -- machine readings previously produced by running virtually every possible experiment.

For one case study, that meant running more than 400 different experiments, said Bier, director of CMU's Center for Molecular Analysis.

"A lot of the data is bad data and that's part of the learning experience," he added.

The experiments can be done much faster in the virtual lab than in real life -- minutes or hours, compared to two days for a real experiment -- so users can quickly learn from their mistakes.

And there's no way for users to break an expensive machine, so there's no harm in fiddling with the machine settings.

Users don't actually prepare the physical specimens -- something that requires standard laboratory technique -- but the Web-based controls for the machines are quite similar to modern mass spec devices, which now are routinely controlled by computers, Grabowski said.

The Pitt and CMU groups have been working on the virtual lab for about four years, sponsored by a \$450,000 grant from the National Science Foundation.

Chunguang Yang, a research assistant in Bier's group, developed a major portion of the software.

The CMU and Pitt groups have been working independently on case studies for the site and eventually hope to have a dozen or more.

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