NATIONAL WATER QUALITY LABORATORY
NEWSLETTER
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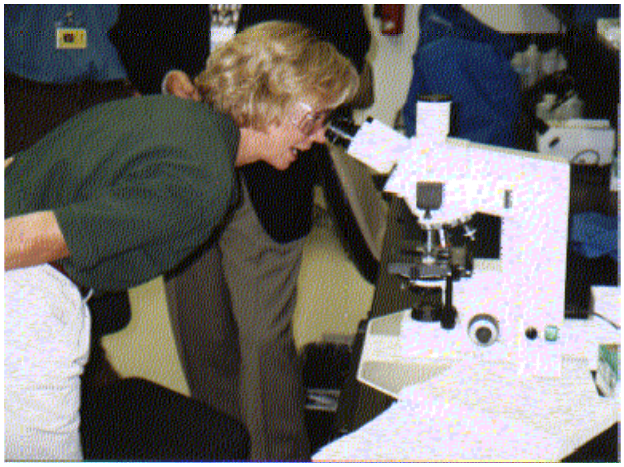
StarLIMS in testing phase

The StarLIMS development team on May 15 began the parallel-testing phase for implementing the new Laboratory Information Management System. All aspects of StarLIMS are being tested, including login, sample preparation, worksheet production, manual result entry, automated results entry, analytical review, quality-assurance checks, data release, billing, and district reanalyses.

Representatives from Automated Data Processing, Login, Inorganic and Organic Chemistry Programs, Quality Assurance Unit, and Administration are taking part in the tests and will help to determine system readiness. Results of the parallel testing will be compiled and evaluated to assess the status of StarLIMS implementation.

Tom Bushly



SMITTEN BY MIDGES-Kathryn Clement, USGS Deputy Director, takes a microscopic view of midges during a tour of the Biological Group labs May 23, at NWQL. Clement was briefed prior to the tour by Lab Chief Greg Mohrman and his Senior Staff.

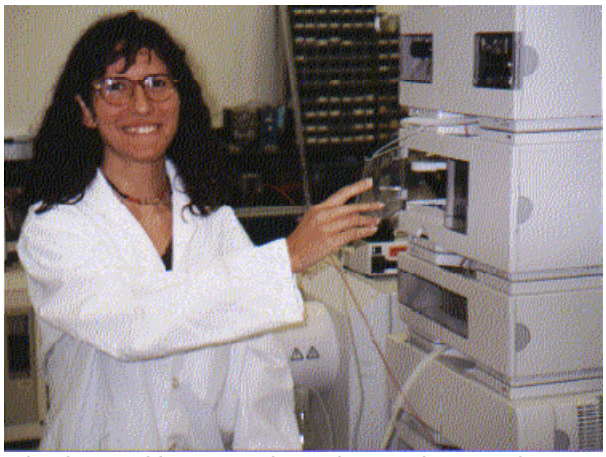
DEPUTY DIRECTOR TOURS LABS-Imma Ferrer (right), postdoctoral research associate, explains one of her projects on pesticides and their degradation products to Kathryn Clement, USGS Deputy Director. Tom Casadevall (center), USGS Central Region Director, escorted Clement on the NWQL tour. Greg Mohrman (behind Casadevall) organized the briefing and tour.

Postdoc from Spain expands NWQL capabilities in high-performance liquid chromatography and mass spectrometry

Dr. Imma Ferrer joined the Methods Research and Development Program at the NWQL in January as a postdoctoral research associate to pursue several areas of analytical chemistry with Ed Furlong, research chemist. During her stay at the NWQL, Ferrer and Furlong are working together to develop and apply new methods for several emerging contaminant classes. This work includes extending the custom analytical method for pharmaceuticals with additional degradation products and new drugs of interest. The method, initially developed by Jeff Cahill and Furlong, has been used as part of a national reconnaissance of emerging contaminants sponsored by the USGS Toxic Substances Hydrology Program.

A second project includes the development of rapid mass spectrometric techniques to identify and quantify pathogens typically found in water samples. This application is being investigated in collaboration with Professor Kent Voorhees and Assistant Research Professor Franco Basile at the Colorado School of Mines in nearby Golden.

The research uses high-performance liquid chromatography/electrospray ionization–tandem mass spectrometry (HPLC/ESI–MS/MS) and matrix-assisted laser desorption ionization/time-of-flight/mass spectrometry (MALDI/TOF/MS). The HPLC/ESI–MS/MS was installed in the Methods Research and Development Program last July and the MALDI/TOF/MS was recently acquired by Colorado School of Mines through a National Science Foundation grant.



RESEARCH INTO NEW ORGANIC CONTAMINANTS-Imma Ferrer, postdoctoral research associate, loads sample extracts into autosampler for analysis by high-performance liquid chromatography/electrospray ionization-tandem mass spectrometry. Dr. Ferrer is helping NWQL develop and apply new methods for emerging contaminant classes. (Also see photo on p. 1.)

Ferrer is also working on projects that apply HPLC/ESI–MS/MS to the detection and identification of pesticides and pesticide degradation products. In collaboration with Jerry Leenheer and Colleen Rostad, National Research Program, Ferrer is also applying HPLC/ESI–MS/MS to determine structural components of fulvic acids. In addition, she is collaborating with Mike Thurman at the U.S. Geological Survey Organic Geochemistry Laboratory in Lawrence, Kansas.

Ferrer received her M.S. (1996) and Ph.D. (1999) degrees from the University of Barcelona, Spain. During her degree program, she worked with Thurman for 2 months while analyzing herbicides at the lab in Lawrence.

Three programs - Toxic Substances Hydrology, the National Water-Quality Assessment, and NWQL Methods Research and Development - are all supporting this postdoctoral research associateship.

Bob Green

PERSONAL TOUCH-Greg Mohrman, newly appointed Chief of the National Water Quality Laboratory, lost no time in emphasizing service and safety, and if they come with a smile, so much the better. Mohrman took up his new post March 27 after serving as Executive Director of the Rocky Mountain Arsenal in Denver. (See NWQL Newsletter, v. 8, no. 2, April 2000, p. 1–3.)

SECRETS OF THE DEEP-Pat Shanks and Lisa Morgan, USGS Mineral Resources Team, presented a talk February 24 entitled "The Floor of Yellowstone Lake Is Anything But Quiet: New Discoveries from Sonar Imaging, Seismic Reflection, and Magnetic Surveys." Recently completed high-resolution surveys of the northern part of Yellowstone Lake show a lake bottom covered with dozens of circular depressions and thousands of spires and pinnacles protruding from the lake floor. The spires, made primarily of silica, are up to 35 meters high and 50 meters in diameter. Morgan and Shanks suggested that the linear features may sit astride fissures on the lake floor. Their research is continuing as they try to understand the geologic processes that shape the lake and how they affect present-day lake populations. They spoke as part of the NWQL Seminar Series.

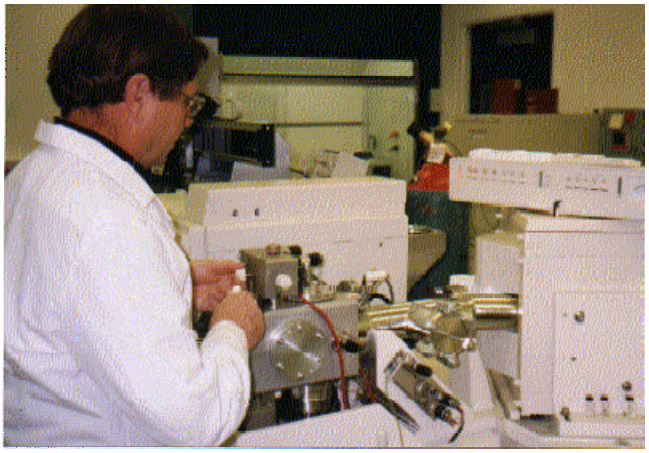
High-resolution mass spectrometry effective for identifying unknown organic compounds in tissue and sediment samples

Organic compounds exist in all living and nonliving matter. They are found in nature and fossil fuels. They are synthesized by man for use as pesticides, insecticides, herbicides, fungicides, pharmaceuticals, detergents, paints, industrial chemicals, and flame-retardants, just to name a few. When these compounds enter the environment, many of them will produce metabolites and degradation products through a variety of biological, chemical, and environmental mechanisms.

For routine or target compound analysis, gas chromatography with low-resolution mass spectrometry (GC/MS) has been used successfully. All of the currently approved GC/MS methods at the National Water Quality Laboratory use capillary gas chromatography with low-resolution mass spectrometry (GC/LRMS).

In environmental analysis, it can be difficult to identify nontarget unknown organic compounds as well as known compounds. The mass spectrum from An environmental sample is compared to mass spectra that are contained in a reference library to identify or confirm the presence of an organic contaminant by using routine GC/LRMS analysis. The compound is considered positively identified if an acceptable match is made with the mass spectrum. If a positive library match is not made, and a positive identification is required, then the extract must be reanalyzed.

In all forms of GC/MS, the molecule that enters the ionization source will be ionized and may be broken down into various fragment ions. The fragmentation path is unique for every organic molecule. Conventional low-resolution mass spectrometry measures the mass of these ions to the first decimal point. High-resolution mass spectrometry measures the mass of these ions to the fourth decimal place. The added accuracy of high-resolution data is used to postulate molecular structures for the unknown or nontarget compound in question.



FINE-TUNING-Chemist Tom Leiker adjusts a high-resolution mass spectrometer prior to injecting a sample extract into the instrument.

In the environment, various combinations of chlorine, bromine, fluorine, phosphorus, and sulfur are contained in many compounds that are present in environmental extracts. The various combinations of these elements at times might make the interpretation of the possible structures of unknown or nontarget compounds difficult. The application of high-resolution mass spectrometry can assist with this task by producing a list of possible empirical formulas. Without these data, it is nearly

impossible to postulate empirical formulas for nontarget compounds that are not contained in a reference library of mass spectra.

High-resolution mass spectrometry is being used to identify unknown compounds that have been detected in tissue and sediment extracts from the National Water-Quality Assessment Program, the endocrine-disruption study on Lake Mead, Nevada, and the Tres Rios Project in Phoenix, Arizona.

For more information on this technique or to inquire how it might be used in projects, contact Tom Leiker, telephone 303-236-3955 or send E-mail to tjleiker.

Tom Leiker

SEAL OF APPROVAL-All floors in storage rooms for warehouse chemicals and for hazardous waste treatment were stripped and sealed the last week of February. Berms to contain potential spills were also added in each storage room. Steve Martin (left) and Joe Santillanes cleaned the storage rooms and helped to apply the second coat of epoxy sealant. They also constructed berms for spill containment in the hazardous waste treatment suite as well as the chemical storage rooms. A final top coat of epoxy and hardener was added to complete the job. The Safety Office says the work was required by the West Metro Fire District codes.

ROBOTIC HANDLING SYSTEM-Charles Patton, Research Chemist in the Methods Research and Development Program, evaluates a prototype robotic liquid sample handling system. It is configured for automatic, simultaneous preparation of digests for dissolved Kjeldahl nitrogen (DKN) and dissolved low-level phosphorus (LLDP) determinations. This prototype system could perform sample- and reagent-dispensing operations needed to prepare one DKN digest and one LLDP digest in about a minute.

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