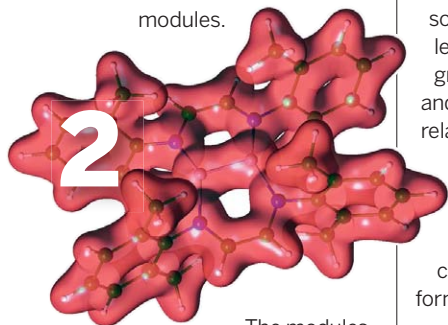


digital briefs

NEW SOFTWARE AND WEBSITES FOR THE CHEMICAL ENTERPRISE

ONLINE

MyLIS (My Laboratory Information System) is a new Web-based, general-purpose management and information system for small, open-access research groups. Each group can create a searchable research profile that aids in locating expertise and resources. The password-protected website integrates key pieces of information that such groups use into a series of modules.



The modules allow groups to track chemicals, supplies, instrument use, orders, and spending; schedule meetings; manage group publications from inception to publishing; assign tasks to group members; and upload or store files and Web links. Designed for ease of use, MyLIS is simple, and in some cases free, to implement, no matter what the field of research. Services range from basic MyLIS (up to 50 MB of storage) to premium accounts (up to 50 GB of storage). The MyLIS website is accessible from any Web-enabled device. **Instras Scientific, www.instras.com**

(1) Linus Pauling and the Nature of the Chemical Bond: A Documentary History is a new website dedicated to one of the 20th century's most illustrious scientists. Composed of three large subsections, the site (osulibrary.oregonstate.edu/special/collections/coll/pauling/bond)

tells the story of the elucidation of chemical-bond theory in a different way. The first section, "Narrative," is a 49-chapter-long account that illustrates the early years of chemical-bond investigation. It focuses primarily on Pauling's research, which Pauling himself later proclaimed to be his most important contribution to science. The second section, "All Documents and Media," provides unprecedented access to more than 300 primary source materials—including letters, manuscripts, photographs, audiovisual materials, and published papers—that relate directly to Pauling's work on the chemical bond. The third section, "Linus Pauling Day-by-Day," consists of a comprehensive account presented in calendar form of all of Pauling's personal

and professional endeavors from 1930 to 1939, when he was writing these seminal papers, and in 1954, when he was awarded the Nobel Prize in Chemistry for his research into the nature of the chemical bond. **OSU Libraries, osulibrary.oregonstate.edu**

SOFTWARE

Thermo Scientific ToxID is software for liquid chromatography coupled with mass spectrometry (LC-MS) analyses. The software is the latest addition to Thermo Scientific's roster of solutions for toxicology and forensic applications, and it is designed to work seamlessly with earlier applications. The software application simplifies LC-MS/MS toxicology screening workflows for toxicology and forensic laboratories, and it uses compound retention

time and MS/MS spectra for confident and accurate compound identification. Pre-defined LC-MS/MS instrument and sample preparation methods are provided to handle several classes of compounds for "General Unknown Screening" analysis. Clear and concise sample reports are generated automatically. The free ToxID software and its compound library are easily customizable and expandable to fit a laboratory's specific needs. The software runs on any Windows-based PC. **Thermo Scientific, www.thermo.com**

(2) Molcas v7.0 is a program package for electronic structure calculations with capability for QM/MM (combined quantum and molecular mechanics modeling). The program enables studies to be performed on many levels of theory, with emphasis on multiconfiguration description, bond formation, and actinide chemistry. The software computes relevant molecular properties (such as chemical structures, frequencies, and activation energies), and it handles relativistic effects explicitly for heavier elements. Molcas (a quantum chemistry code that allows studies of molecular systems using a variety of quantum chemical models) runs on Mac, Windows XP, and Linux. **Lund University, www.molcas.org**

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You go girl! Informative website for future female engineers

A recently launched website is encouraging girls to enroll in undergraduate engineering. The WGBH Educational Foundation and the National Academy of Engineering, with help from more than 50 other organizations, aim to have **www.engineeryourlife.org** serve as a guiding resource of information, a forum for collaboration, and a catalyst for inspiration to spur girls into engineering. The site includes the stories of 12 women and how they came to choose engineering as a profession, detailed descriptions of 11 engineering fields, and a how-to section on preparing for college including details on what high school classes to take and what aspects of engineering programs to look for. **NAE, www.nae.edu; WGBH, www.wgbh.org**

