

Happy Holidays to you and your families from the Computational Chemistry Communiqué!

People on the Move

Atul Agarwal, formerly with Wyeth Pharmaceutical Research, has recently accepted the position of Director, Computational Chemistry and Informatics at Achillion Pharmaceuticals.

Erin Bradley, formerly with DeltaGen, has accepted the position of Associate Director, Computational Chemistry at Sunesis Pharmaceuticals.

Chaya Duriaswami, formerly with Pharmacoepia, has moved to GlaxoSmithKline as an Investigator in the Structural Chemistry group.

Peter D. J. Grootenhuis, formerly with DeltaGen, has accepted the position of Senior Director, Computational Chemistry and Lead Discovery at Vertex Pharmaceuticals.

Ravi Jalluri has recently left Signal Pharmaceuticals to accept the position of Group Leader, Computational Chemistry at Genome Therapeutics Corporation.

Adam Kallel, formerly with Elitra, has joined Ligand Pharmaceuticals as a Senior Scientist in Computational Chemistry.

Tudor Oprea has recently moved from AstraZeneca, Mölndal to the Office of Biocomputing at the University of New Mexico School of Medicine.

Carlton Sage, Formerly with Lion Bioscience, has recently joined the computational chemistry group at Arena Pharmaceuticals as a senior computational chemist.

New Technology

TurboGenomics (www.turbogenomics.com) has announced the immediate availability of TurboBench 2.0, an application software platform that delivers previously unattainable levels of speed and automation for computational workflows common in drug discovery and throughout the industry. TurboBench 2.0 enables users to exploit all of the computing power available on heterogeneous mixtures of multiprocessor servers, clusters, networked desktops, and computational grids without rewriting current applications. The parallel and distributed computing technology that underlies TurboBench 2.0 makes it possible for users to complete jobs in just a few minutes instead of the hours or days required previously.

Molecular Networks GmbH (www.mol-net.de) has announced a new program called CLIFF for the interconversion of more than 40 different chemical structure exchange file formats. CLIFF supports most of the commonly used formats for chemical compounds (SMILES, SDF, MOL, MOL2, ...) and reactions (RXN, RDF). CLIFF (Chemical Libraries - Interconversion of File Formats) is a powerful program which provides a series of functionality, which goes beyond a simple conversion tool:

- generation of 2D coordinates by a state-of-the-art 2D structure layout module of the CACTVS system licensed from Xemistry GmbH
- template-based 2D structure arrangement
- enrichment of datasets with additional information, such as molecular weight, number of H-donors, etc.
- automatic hydrogen addition or removal
- features for the removal of counterions in salts

Advanced Chemistry Development (www.acdlabs.com) has posted the Public Chromatography Applications Database under their web-based analytical data delivery tool, ACD/Web

Librarian. A free trial of ACD/Web Librarian and access to the Public Chromatography Applications Database is available through their interactive laboratory tool, ACD/I-Lab, at <http://www2.acdlabs.com/ilab/>.

The Public Chromatography Applications Database, excerpted from ACD's Chromatographic Applications Database, contains 1830 HPLC and GC applications provided by Agilent, Alltech, Eprogen (Eichrom), GL Sciences, Hamilton, Argonaut (Jones Chromatography), Polymer Laboratories, and Regis. The database can be searched by numerous chromatographic parameters, as well as by structure, substructure, and structure similarity.

The Career Corner

As anyone who monitors employment in the pharmaceutical and biotechnology industries can attest, 2002 has been a tough year. According to data from the Bureau of Labor Statistics, employment in the "Drugs" sector has remained relatively steady at around 329,000 employees ($\pm 3,000$). However, press releases from the industry during the third and fourth quarters have reported the elimination of over 1,100 early stage research positions. In this environment, it is important to keep your resume up-to-date, maintain contact with the people who will serve as your references, and have a seminar available that will highlight your skills and accomplishments.

As a first step, take a critical look at your resume. While it is important to have your patents and publications current, it is also time to delete items that are not germane to your current experience level - e.g., the internship that you held during the summer of 1986. Remember to keep it brief. If you use more than two - three pages, excluding publications, you can probably start trimming.

Once your resume is in shape, it is time to think about a seminar. During twenty-three years of working in, and with, the pharmaceutical industry, we have attended every type of seminar imaginable - technical, sales, infomercial, etc. These have been presented by scientists ranging from experienced managers to graduate and postdoctoral students who are interviewing for their first jobs. As you might expect, the quality of these presentations has ranged from good to bad to indifferent. The one point that has always distinguished a good seminar however, regardless of the purpose, was that it told a story in a logical, stepwise manner. In addition, your seminar should be:

- **Concise.** Rather than attempting to highlight every technique you have used during your career, develop one theme that shows how your skills impacted a specific project. Remember that you have 45 minutes

to present your material. Given that the average slide takes 1 - 2 minutes to present, your seminar should have no more than 30 slides.

- **Legible.** If your slides are packed with so much information that people at the back of the room cannot read them, you have lost your audience. Summarize tables of data rather than showing all of the entries.

- **Entertaining.** People want to hear about your work, not have you read it to them. Use bullets as talking points and remember to vary your tone of voice during the presentation.

- **Diverse.** Historically, computational chemists have presented to colleagues. However, this no longer the anticipated audience. Committees comprised of medicinal chemists, biologists, informaticians, and computational chemists now make hiring decisions. Your presentation should include material that is of interest to each of these disciplines.

Until recently, computational chemistry groups were rarely hit with the staff reductions seen in other research disciplines. Generally, the total number of CADD employees continued to grow even though there have been periods of time when group size was held constant. However, given recent shifts in research priorities, mergers, and corporate valuations, it is prudent to be prepared to quickly initiate a job search if conditions at your company change.

Contact Information

If you have information that you would like to post or topics you would like to see addressed, please contact Merry Ambos. The Computational Chemistry Communiqué is published quarterly by Molecular Solutions. If you would like to receive C³ via email as a pdf file or you would like to have your name removed from our mailing list, please email Merry at mambos@molsol.com.