

Introduction

Welcome to the Computational Chemistry Communiqué! This quarterly publication is designed to keep the CADD/CAMM community up-to-date on the latest news. Regular features will include **People on the Move**, brief descriptions of **New Technology**, and **Career Corner**. 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.

People on the Move

Markus Boehm, who recently graduated from the University of Marburg, has joined the Computational Chemistry Department at Pfizer Global Research and Development in Groton as a Research Scientist.

Mike Bower has moved from GlaxoSmithKline to Incyte Pharmaceuticals as a Principal Research Scientist in Computational Chemistry.

Matthew Clark has accepted the position of Director of Research Information Technology at Locust Discovery Technologies.

Erin Duffy, formerly with Achillion Pharmaceuticals, has accepted the position of Director, Structure-Based Drug Discovery at Rib-X Pharmaceuticals.

Sergio Rotstein, formerly with Vertex Pharmaceuticals, has accepted the position of Senior Investigator, Informatics & Modeling at ArQule, Inc.

Dominic Ryan, formerly with GlaxoSmithKline, joined Millennium Pharmaceuticals as the Associate Director of Computational Chemistry.

Clayton Springer, recently a postdoctoral fellow at Sandia National Laboratories, has joined the Novartis Biomedical Research Institute as a Senior Scientist in Biomolecular Modeling.

New Technology

Direct Force Field is a novel program for molecular mechanics from *Aeon Technology* (<http://www.AeonTechnology.com>). Its most unique feature is that it can be used to build molecular mechanics force fields automatically when existing force fields are insufficient or inaccurate. A patent-pending process enables fast and reliable parameterization from *ab initio* data. In its latest release (version 1.2), this product has been extended to support nonbond parameterization using thermophysical data of condensed matters. Other force field-related features implemented in this product include parameter estimation, as well as the capability to convert parameters from one force field type to another. This product can be used for energy minimization and molecular dynamics simulations.

InforSense (<http://www.inforsense.com>) is a leading provider of discovery informatics software and services for the life science industry. Our expertise is in the development of high performance enterprise-wide discovery planning systems, which combine flexible knowledge management, large-scale data mining, analysis and visualisation. InforSense's flagship product, Kensington Discovery Edition (KDE), is an advanced informatics platform designed to support large-scale information-driven discovery in life sciences. Its open architecture allows for comprehensive, flexible functionality including multi-source data integration, powerful data analysis and visualisation, intuitive process management, and efficient collaboration support, all at an enterprise level. KDE and its life science components support the requirements of the entire discovery life cycle and effectively increase the productivity of life science research.

BioRelation (<http://www.biorelation.com>) has released PharmTree, a Web-based structure classification, activity, toxicity prediction and active pharmacophore identification system that fingerprints and classifies a large number of chemical compounds according to their biological response data. Coupled with a Web-based chemical structure server, it automates millions of calculations giving scientists an

easy-to-use interface. The system is designed for bench scientists and computational chemists.

The Career Corner

This section of C³ will highlight trends in computational chemistry hiring, salaries, group size and budgets. Additionally, we will write short articles covering topics such as career management and job strategies.

What is the current US job market for computational chemists? It depends on where you find your data. The most recent report from the Bureau of Labor Statistics shows that 330,700 people were employed in the "Drugs" sector of the US work force as of June 2002. This is an increase of 9,000 full-time positions compared to the same period in 2001.

In contrast to these statistics, articles in several industry publications state that companies in the "genomic" sector have downsized by a total of 1,500 positions. Most of these reductions have been made in the "tools and technologies" (i.e., programming and databases) sector of the industry. In the biopharmaceuticals segment, companies have responded to the shrinking availability of new capital by reducing headcount and outlicensing promising projects. Through June, several companies reported staff reductions of over 500 positions.

For computational chemistry, the current status is mixed. Three organizations eliminated positions in computational chemistry over the first half of the year. However, during this same period fifty-six openings for computational chemistry and cheminformatics were advertised. While many of these positions were filled, over a dozen remain open. It appears that the overall number of computational chemistry jobs is not decreasing, however, the market is in a state of flux. As a result, rather than looking for a computational chemist with a general set of skills, many companies have very specific requirements for their openings. As a result, job seekers should make sure that their resume is tailored to each company to which they are applying.

While the number of openings within computational chemistry continue to vary each year, salaries have consistently increased. According to recent surveys conducted by Molecular Solutions, over the last five years the average salary for entry level computational chemists at smaller biotech and pharmaceutical companies has increased by over 23%. At larger companies, the average starting salary has increased by over 33%. For positions requiring three to five years of experience, the average salary at smaller companies has increased by 37% while larger

organizations show an increase of 46%. In the six to eight years of experience band, the increases are 36% and 30% for smaller and larger companies respectively. As stated above, requirements for these positions have also increased in scope with most companies now requiring postdoctoral training and some relevant industry experience. Several groups also require experience in object oriented software development.

The average size of computational chemistry groups also has grown over the past six years. Comp groups in smaller organizations averaged three modelers in 1995 and four at the end of 2001. In larger organizations, the average number of computational chemists increased from eight in 1995 to eighteen in 2001, an increase of 125%.

About Molecular Solutions

Founded in 1992, Molecular Solutions (<http://www.molsol.com>) is the only professional placement firm working exclusively in the areas of computational chemistry, scientific programming, and cheminformatics. The founders of the company, Allen Richon and Merry Ambos, each has over twenty-five years experience in these areas. As a result, Molecular Solutions has both the technical background and the industrial experience required to effectively assist chemical, biotechnology, and pharmaceutical research organizations in locating and hiring research scientists for their computational chemistry openings. For assistance with your next job search, or for more information on placement services from Molecular Solutions, please contact us at 843-886-8775 or e-mail us at mambos@molsol.com.

About Network Science

Founded in 1995, Network Science (<http://www.netsci.org>) is a 501(c(3)) non-profit organization with the mission of promoting careers in pharmaceutical research and providing continuing education resources to research scientists. As a part of its mission, Network Science conducts surveys on trends in pharmaceutical research, the application of technology to drug discovery and career development for research scientists.