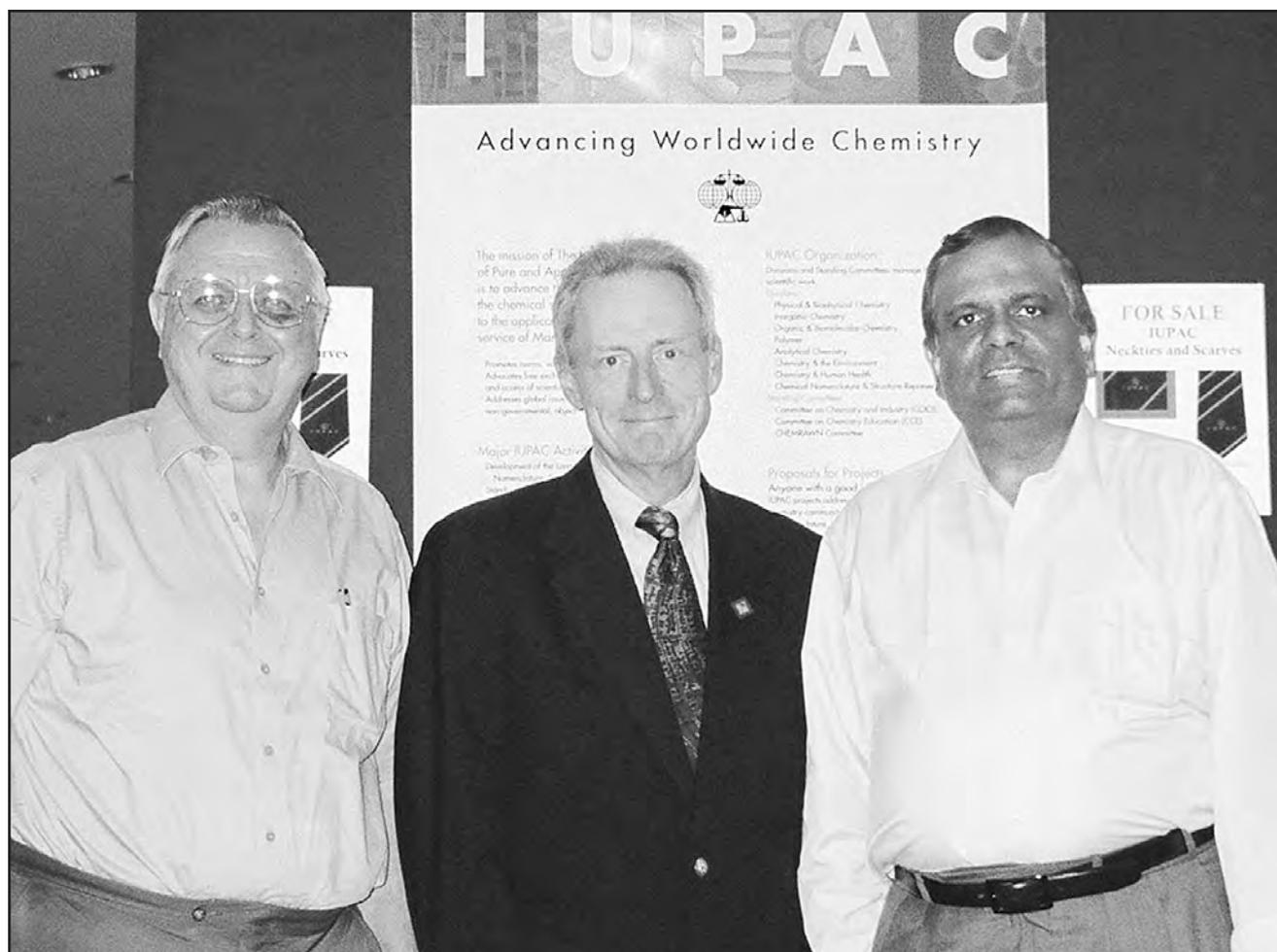


THE NUCLEUS

December 2005

Vol. LXXXIV, No. 4



Monthly Meeting

Medicinal Chemistry Symposium on Type 2 Diabetes

2005 IUPAC Congress and General Assembly

Report by Morton Z. Hoffman

Tailoring the Analytical Chemistry Effort

By Martin Freier

Management of Biological Data

By Mustaq Ahmed, et al. and Mukund Chorgade

Report From China: IUPAC Congress and General Assembly

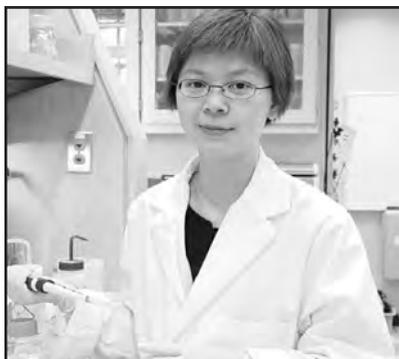
Morton Z. Hoffman,
Boston University, U.S. National Representative to the IUPAC Committee on
Chemistry Education, Division of Chemical Education, Liaison to IUPAC

The 40th IUPAC World Chemistry Congress (*Innovation in Chemistry*) and the 43rd IUPAC General Assembly were held concurrently at the Beijing International Convention Center, August 14-19, 2005. The Congress, which was organized by the Chinese Chemical Society and the Institute of Chemistry, Chinese Academy of Sciences, was a general scientific meeting, not unlike an ACS meeting, while the General Assembly was the occasion for meetings of the governing bodies and committees of the Union such as the Committee on Chemistry Education (CCE).

Mukund Chorghade (Associate Member of CCE, President of D&O Pharmachem, 2006 NESACS Chair-Elect) and I attended the meetings of CCE, where there was much discussion about the recent directive from the Chinese Ministry of Education that would require the teaching of science and mathematics in China's many colleges and universities in English within a very short time, and as little as three years for the most prominent institutions. It was announced that the 19th International Conference on Chemical Education (ICCE) will be held in Seoul, Korea, August 12-17, 2006; for more information, see <<http://www.19icce.org>>.

Eight young chemists, two of whom have ties to institutions within NESACS, were honored by IUPAC at the Congress with the 2004 and 2005 prizes.

Yu Huang received her Masters and Ph.D. degrees in Chemistry from Harvard University, and her Bachelor's degree from the University of Science and Technology of China. Dr. Huang is now a Lawrence Fellow working in the Biomolecular Material Laboratory at the Department of Material Science



Dr. Yu Huang (2004 IUPAC Prize for a Young Chemist)



Dr. Zev Gartner (2005 IUPAC Prize for a Young Chemist)

and Engineering, Massachusetts Institute of Technology. She has made profound contributions to the field of nanoelectronics with her inventions: methods for bottom-up assembly of nanoscale electronic and optical devices and circuits using chemically synthesized nanowires as building blocks. Her thesis is entitled *Integrated Nanoscale Electronics and Optoelectronics: Exploring Nanoscale Science and Technology through Semiconductor Nanowires*.

Zev Gartner received his B.S. in chemistry from the University of California at Berkeley in 1999. He performed his doctoral work at Harvard

Call For Nominations

*International Union of Pure
and Applied Chemistry*

IUPAC announces the **2006 IUPAC Prize for Young Chemists**. The IUPAC Prize for Young Chemists has been established to encourage outstanding young research scientists at the beginning of their careers. The prize will be given for the most outstanding Ph.D. thesis in the general area of the chemical sciences, as described in a 1000-word essay. Prize is USD \$1000 and travel to the IUPAC Congress in Turino, Italy, August 2007. Each awardee will be invited to present a poster on his/her research and to participate in a plenary award session.

Call for Nominations: (deadline February 1, 2006)

For more information, including application form, please visit the IUPAC web site at

www.iupac.org/news/prize.html

or contact the IUPAC Secretariat by e-mail at <secretariat@iupac.org>

or by fax: +1 919 485 8706 ◇

University, receiving his Ph.D. in June, 2004. After several months working as a research consultant for a start-up company in Cambridge, MA, followed by a half year of world travel, he recently began his post-doctoral work at Berkeley with Professor Carolyn Bertozzi. Zev's Ph.D. thesis, entitled *The Development of DNA-Templated Organic Synthesis*, was completed under the supervision of Professor David Liu.

Among the plenary speakers at the Congress was William Lipscomb (Harvard University) who spoke on "Structure and Functions in Chemistry and Biology - Experimental and Computational Studies." I chaired a session in the chemical education program and presented a contributed paper on "Increasing the Yield of Chemistry Students in the United States." ◇

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Cover: (l-r) Morton Hoffman (Boston University), Bill Carroll (ACS President), Mukund Chorghade (President of D&O Pharmachem) at the 40th IUPAC World Chemistry Congress and the 43rd IUPAC General Assembly, Beijing, China, August 14-19, 2005.

Deadlines: *February Issue: December 9, 2005*

March Issue: January 13, 2006

THE NUCLEUS

The Nucleus is distributed to the members of the Northeastern Section of the American Chemical Society, to the secretaries of the Local Sections, and to editors of all local A.C.S. Section publications. Forms close for advertising on the 1st of the month of the preceding issue. Text must be received by the editor six weeks before the date of issue.

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Tailoring the Analytical Chemistry Effort

By Martin Freier

Analytical chemists gather information regarding compounds, using a host of sophisticated tools; analyze that information; and report their findings. In a sense, they serve as the auditors in the chemical industry by identifying any deviations from standards. Unlike the auditors, however, analytical chemists also provide the chemical industry with insight into newly synthesized compounds and thus allow company managers to make some major strategic business decisions regarding the production, distribution, and application of such compounds. At the same time, they also help government regulatory agencies to implement appropriate measures required for assuring safety and quality to the public.

Since it is crucial that the information gathered be as accurate and as timely as possible, in some cases robotic real-time instrumentation is now used to assure quality and safety of certain processes and is thus replacing analytical chemists. Oddly enough, these instruments and their application are designed by the analytical chemists being replaced in the process. They are aware that the required sophisticated tools and qualified scientists who are able to use them are in many cases not as widely available as dictated by established schedules, budgets, and safety concerns (areas where it would be hazardous to use human operators for real-time quality control). Analytical chemists often resort to sampling and statistical methods to reduce costs and schedules, where possible. Other effective means, such as outsourcing of the work to qualified sources outside the company, are now among the effective strategies being implemented. In short, one of the major challenges chemists face daily is how best to implement the analytical chemistry effort of the project in a timely and cost-effective manner.

Howard Jordi, PhD, CEO of Jordi

FLP, a Massachusetts based laboratory (Bellingham), has been in the analytical chemistry field for more than 25 years and believes that each of the strategies used to implement analytical chemistry should be considered. He is a proponent of tailoring the analytical chemistry work to the specific problem. Each chemical problem is unique, and the analytical chemistry needs must be separately assessed and a determination made as to how best to address that problem before proceeding. But ultimately, the decisions on how much analytical chemistry must be authorized has to be made by the chemists and the regulatory agencies who have the unique expertise and the full responsibility.

When Jordi was pursuing his Ph.D. studies at the Northern Illinois University's biochemistry laboratory, his doctoral thesis was enzyme kinetics. In those days, he considered himself a biochemist who loved to synthesize chemical compounds. After spending several years at the Walter Reed Medical Center Research facility and Waters' Associates Laboratory, he realized that he enjoyed analytical chemistry. Indeed, Jordi is a biochemist who at a point in his career decided to specialize in analytical chemistry. Many scientists have made similar choices.

Given his successful career in synthesizing compounds, why did Jordi choose analytical chemistry?

"First, believe it or not, I just enjoyed analytical chemistry's highly structured methodology, which still allows the chemist a great deal of creativity, especially with analyzing the new complex compounds being synthesized; besides, there is a great deal of synthesis going on in analytical chemistry."

What Jordi was alluding to was the fact that there is quite a bit of synthetic chemistry involved in the columns used in chromatography.

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Some of the many creative tasks analytical chemists perform these days include designing the processes and the instrumentation and computer programs required. What is amazing is the complexity of some of the instruments and computer programs the analytical chemists are involved in. Nowadays some of them are spending a great deal of time in designing the sensors and instrumentation for detecting explosives and radioactive materials as a means for dealing with potential terrorist threats. Other applications include closed-loop automation systems based on spectroscopy that use in-line fiber-optic probes to gather information and facilitate quick comparisons with existing spectrum profiles and thus assess deviations from acceptable standards

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Monthly Meeting

The 865th Meeting of the Northeastern Section of the American Chemical Society

Jointly with the Medicinal Chemistry Group

Symposium: Diabetes II, part II.

Thursday – December 8, 2005

Holiday Inn Select – Woburn, MA - 15 Middlesex Canal Park Road

3:00 pm Refreshments

3:15 pm Welcome, Raj (SB) Rajur, Program Chair

3:20 pm Introductory Remarks, Norton Peet, North Andover, MA

3:30 pm *Applying RNAi and Structure-Based Medicinal Chemistry for Treatment of Obesity and Type II Diabetes*
Mark Tepper, CytRx Corporation, Worcester, MA

4:30 pm *Development of DPP4 Inhibitors Using High Throughput Crystallography*, G. Sridhar Prasad, Merck & Co., Inc., West Point, PA

5:30 pm *TBA* Subramanyah Hosahalli, Aurigene Discovery Technologies, Bangalore India

6:30 pm Social Hour

6:45 pm Dinner

7:45 pm *The Story of Vildagliptin (LAF237): A DPP4 Inhibitor for the Treatment of Type 2 Diabetes*. Edwin B. Villhauer, Novartis Pharmaceuticals, East Hanover, NJ

Dinner reservations should be made **no later than 12:00 noon on Thursday, December 1, 2005**. If you prefer to pay at the door, please contact Marilou Cashman at (800) 872-2054 or (508) 653-6329 or mcash0953@aol.com. Reservations not canceled at least 24 hours in advance must be paid. Members, \$28.00; Non-members, \$30.00; Retirees, \$15.00; Students, \$10.00. Anyone who needs handicapped services/transportation, please call a few days in advance so that suitable arrangements can be made.

Directions to Holiday Inn Hotel - <http://www.radisson.com/woburnma>

From Boston - Cambridge - Points North: Take Route I-93 to Route 95/128 West. After 1 mile, take Exit 35 South to Route 38 (Main Street).

***After about 500 feet at the traffic light, turn right into Middlesex Canal Street to the hotel entrance.**

From the West: Take Route 95/128 North to Exit 35 South (Route 38 - Main Street). **Follow directions from * above.**

THE PUBLIC IS INVITED

Abstract:

The Story of Vildagliptin (LAF237): A DPP4 Inhibitor for the Treatment of Type 2 Diabetes

Dipeptidyl peptidase IV (DPP4) inhibition has the potential to become a valuable therapy for type 2 diabetes. The synthesis and structure activity relationship of a new DPP4 inhibitor class, N-substituted-glycyl-2-cyanopyrrolidines, are described as well as the path that led from clinical development compound 1-[2-[5-cyanopyridin-2-yl]amino]-ethyl-amino]acetyl-2-cyano-(S)-pyrrolidine (DPP728) to its follow-up, 1-[[[3-hydroxy-1-adamantyl]amino]acetyl]-2-cyano-(S)-pyrrolidine (Vildagliptin, LAF237). The pharmacological profile of Vildagliptin in obese Zucker fa/fa rats along with pharmacokinetic pro-file comparison of DPP728 and Vildigliptin in normal cynomolgus monkeys and humans is discussed. The results suggest that Vildagliptin is a potent, stable, selective DPP4 inhibitor possessing excellent oral bioavailability and potent antihyperglycemic activity with potential for once-a-day administration. The results from recent clinical studies will be discussed during the meeting.

[1] Villhauer, E.B.; Brinkman, J.A.; Naderi, G.B.; Burkey, B.F.; Dunning, B.E.; Kapa, P.; Mangold, B.L.; Russell, M.E.; Hughes, T.E. 1-[[[3-Hydroxy-1-adamantyl]amino]acetyl]-2-cyano-(S)-pyrrolidine: A Potent, Selective, and Orally Bioavailable Dipeptidyl Peptidase IV inhibitor with Antihyperglycemic Properties. *J Med. Chem.* **2003**; *46*, 2774-2789. ◇

Biography:

Currently Dr. Villhauer is a Principal Fellow in Process Research at Novartis Pharmaceuticals in East Hanover, New Jersey. Until the move of Novartis Research to Boston in 2003, he worked for over 17 years as a medicinal chemist in preclinical asthma, cardio-

vascular, obesity and diabetes programs at Sandoz and then Novartis in New Jersey as well as Basel, Switzerland. He has led, and championed numerous diabetes and obesity programs while specializing in protease inhibition and combinatorial chemistry. Due to his inventions of Novartis's two diabetes development compounds in the DPP4 inhibitor field (DPP728 and

its successor, LAF237), he was recently awarded the title of Novartis Leading Scientist. He is the author of over two dozen publications and inventor of 9 issued US patents. Dr. Villhauer received his B.S., M.S., and Ph.D. from the University of Rochester. ◇

Call for Nominations

James Flack Norris Award for Outstanding Achievement in the Teaching of Chemistry

Nominations are invited for the 2006 James Flack Norris Award for Outstanding Achievement in the Teaching of Chemistry. The Norris Award, one of the oldest awards given by a Section of the American Chemical Society, is presented annually by the Northeastern Section. The Award consists of a certificate and an honorarium of \$3,000.

Nominees must have served with special distinction as teachers of chemistry at any level: secondary school, college, and/or graduate school. Since 1951, awardees have included eminent and less widely-known but equally effective teachers at all levels.

The awardee for 2005 was Professor Morton Z. Hoffman of the Department of Chemistry of Boston University.

Nominations should focus on the candidate's contributions to and effectiveness in teaching chemistry. The nominee's curriculum vitae should be included. Seconding letters are also an

important part of a nominating packet. These may show the impact of the nominee's teaching in inspiring colleagues and students toward an active life in chemistry and/or related sciences, or may attest to the influence of the nominee's other activities in chemical education, such as textbooks, journal articles, or other professional activity at the local or national level.

Materials should be of 8½ by 11 inch size. The nomination packet should not exceed thirty pages and should not include books or reprints or software.

Please direct questions about the content of a nomination to Professor Marietta Schwartz, University of Massachusetts, Boston, e-mail: Marietta.Schwartz(at)umb.edu. For more information about the Norris Award, see www.nesacs.org.

Send nomination packets (as hard copy, or electronically in Adobe PDF format) to Ms. Marilou Cashman,

NESACS, 23 Cottage St., Natick, MA, 01760. email: [mcash0953 \(at\)aol.com](mailto:mcash0953@comcast.net).

The deadline for nominations is April 15, 2006. ◇

Call for Nominations

Philip L. Levins Memorial Prize

Nominations for the Philip L. Levins Memorial Prize for outstanding performance by a graduate student on the way to a career in chemical science should be sent to the Executive Secretary, NESACS, 23 Cottage St., Natick, MA 01760 by **March 1, 2006**.

The graduate student's research should be in the area of organic analytical chemistry, and may include other areas of organic analytical chemistry such as environmental analysis, biochemical analysis, or polymer analysis.

Nominations may be made by a faculty member or the student may submit an application. A biographical sketch, transcripts of graduate and undergraduate grades, a description of present research activity, and three references must be included. The nomination should be specific concerning the contribution the student has made to the research and publications (if any) with multiple authors.

The award will be presented at the May 2006 Section Meeting. ◇



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Integration and Management of Biological Data for Clinical and Functional Inference; Persistent's Solutions

Mushtaq Ahmed*, Saurabha Daniel*, Armaity Davierwala, Prashant Lele, Ghana Pendse, Aditya Phatak and Prabhakar Ranjekar, Persistent Systems, Pvt. Ltd., Bhageerath, 402, Senapati Bapat Road, Pune 411016, India. www.persistent.co.in and Mukund S. Chorghade, Chorghade Enterprises, 14 Carlson Circle, Natick, MA 01760-4205, USA chorghade@comcast.net

Introduction

The pharmaceutical sector has traditionally been a vibrant, innovation-driven and highly successful component of industry at large. In recent years, a confluence of spectacular advances in chemistry, molecular biology, genomic and chemical technology and the cognate fields of spectroscopy, chromatography and crystallography have led to the discovery and development of numerous novel therapeutic agents for the treatment of a wide spectrum of diseases. Multi-disciplinary and multi-functional teams focusing on lead generation and optimization have replaced the traditional specialized research groups. To develop a drug, from conception to commercialization, the biotechnology / biopharmaceutical industry (which has been highly entrepreneurial) has reached out to establish global strategic partnerships with numerous companies.

Biological research, particularly the genome-sequencing projects allied to drug development is continually producing voluminous data that need to be organized, analyzed and queried to generate useful scientific knowledge. There has been an unprecedented explosion in the number and size of public data resources, and variety and volume of laboratory data.

Challenges

As biological research is being transformed from purely experimental to information-driven discovery science, academia, pharmaceutical, biopharmaceutical and biotechnology

companies are faced with a growing need to integrate proprietary biological data with public data sources across all life science domains. The biggest challenge today is not just to maintain, but semantically integrate genomic and clinical data, enabling researchers to discover relationships and decipher patho-physiological process for better understanding of disease mechanisms and more accurate decision-making for selecting drugs and targets.

The most striking feature of life sciences data is not its volume, but its diversity. Each data source contains a different subset of biological knowledge. There are many integration challenges, as the data sources are dynamic and the data are heterogeneous. The technical challenge is increased with different databases using different DBMS's and ways of data access. Even more challenging is the task of keeping pace with the continual changes and updates of biological data sources, making integration an ongoing task. Finally, intensive research of data content and formats and integration of data sources is a time consuming and tedious effort.

Integration Approaches

There is no single product that addresses the issue of data integration in totality. Typically, groups have utilized three different approaches to solve biological data integration problems in biology. These include Indexed Data Sources (Linked Integration), Federated databases (View Integration), and Data Warehouses / Data Marts.

Indexed data sources or Linked Integration

Linked Integration enables researchers to begin their query search with one data source and then follow hypertext links to related information on other data sources, facilitating interactive browsing. This approach is especially well suited to explore the data landscape when an investigator has not yet formulated a specific question.

Indexed data sources are a variation of linked integration. In this approach multiple data sources are indexed and then linked to support quick queries for customized querying.

This approach is embodied in a popular tool, Sequences Retrieval System [SRS] (Etzold and Argos 1993). It was originally developed by an EBML scientist, and exclusive license rights were later acquired by Lion Biosciences. It is a key word index and searching system for biological databases and supports flat file, relational databases and object-oriented databases also. SRS uses specialized parsing language for generating database wrappers and another specialized language for formulating queries.

Federated Databases

Federated databases provide view integration. Data federation does not modify the primary data source and does not permit replication or migration to a central source. The primary data source remains autonomous, but builds an environment around the databases that makes them all seem to be part of one large system. The middle-

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Management of Data

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ware creates a logical view of the federated databases. Applications interacting with the middleware are presented with a unified schema even though the actual schema is distributed across the data sources. Middleware leverages the native data management and search capabilities; at the same time the wrapper encapsulates the specificity of each database. Searches submitted to the federated middleware are partitioned into sub-queries that can be executed by individual databases. Examples of federated systems include complex-relational systems like BioKleisli/ K2 (S. Davidson, et al.1996), GeneticsXchange's K1, object-relational systems (OPM/TINet) and IBM's relational system DiscoveryLink (Haas, Schwarz et al. 2001).

Data Warehouses and Data Marts

The data warehouse approach assembles data in a centralized system with a global data schema. A data warehouse stores highly redundant

data that is modeled through a multidimensional approach. An indexing system is used for integration and navigation. It is a relational database optimized for pre-defined types of searches. Data marts are smaller, focused data warehouses designed for specific search requirements. Data warehouses are populated from primary data sources, using a three-step process: (a) The data are extracted from primary data source and cleaned, (b) transformed, and (c) loaded into the database and indexes are built to achieve optimum query performance. Data warehouses offer the advantage of mature and widely accepted RDBMS technology and a high-level standard query language (SQL). These systems have been successfully implemented in commercial health care enterprises.

Persistent's Solutions

The interplay of all the challenges in data integration necessitates careful problem definition, requirement gathering and analysis to select the most optimum integration model. Persistent Systems has developed data manage-

ment and integration solutions for functional genomics (proteomics and micro array) at The School of Medicine, Washington University in St. Louis and data integration solutions for the sequencing pipeline at MIT-Broad Institute for Genome Research.

Data Warehousing Solutions for Functional Genomics

At Washington University, School of Medicine, the requirement was to integrate data located at four different cores and stored in different forms:

- Microarray core
- Sequencing core
- Tissue Procurement core
- Proteomics core.

The major design considerations include:

- Fast querying of data from multiple sources.
- Efficient handling of large amounts of data, allowing users to upload and analyze it.
- Provide access to data via a campus-wide intranet for approximately 200 concurrent users.
- In addition, while the experimental data generated within the core facilities is required to be accessed in almost real time, the annotation data coming from publicly available databases needs to be up to date only within the past few weeks.

We chose to use the data warehousing model to store the experimental and annotation data sets. This model allows investigators to collect, download and manipulate large amounts of microarray, gene annotation, gene sequence, reference sequence and 2-D gel data from the University core facilities and integrate it with publicly available data sources providing real-time annotation to expression data in context of gene annotation including Gene Ontology categories, tissue specificity, metabolic and signal transduction pathways, published literature and orthologous sequences through web-based and desktop client applications.

The analysis tools we have developed and deployed help in capturing, inte-

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Management of Data

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grating, sharing, and visualizing post-genomic microarray, proteomics, gene annotation and clinical data. All these solutions provide an integrated query environment.

Our data warehouse runs on Oracle 9i (version 9.2.0.4- 64 bit) database, which is hosted on a Sun Enterprise 420R consisting of 4 X 450 Mhz Ultra Sparc-II processors, 4 GB of internal RAM memory, 36 GB of mirrored internal drive space, and two Sun Stor Edge A1000 RAID boxes, containing 654 GB of total disk space set up to operate in RAID 5 mode. The warehouse currently has about 150 GB of data.

LIMS for Microarray

LIMS for Microarray is used at the Bioinformatics core at Washington University. It is designed to realistically capture every step in a typical microarray facility and provide a complete solution for the management of microarray experiments within a secure environment. LIMS for microarray facilitates organization, storage, archiving and retrieval of all experiment-related information.

Investigators can submit samples on line using a web-based sample submission form. Once the samples are received, the curator can create and enter metadata about new experiments, investigators, samples and chips. Using LIMS graphical interface, the curator can also view, edit or update existing information.

The samples can be tracked by assigning auto-generated unique sample IDs. Barcode labels can be printed for samples to facilitate sample tracking. On completion of an experiment, data files can be uploaded to the database after which an intimation mail will automatically be sent to the investigator notifying him/her that the data have been successfully uploaded/archived on server. The investigators can retrieve the results through a web interface. The results can be analyzed using Function Express gene annotation tool or exported in a simple text

format suitable for import into downstream analysis tools like GeneSpring/Spotfire.

Function Express Gene Annotation Server

The gene annotation server annotates probes on microarrays, using publicly available biomedical databases, and automatically updates these annotations on a regular basis.

Microarray technology allows simultaneous study of expression of thousands of genes, generating large amount of complex data. While analyzing the microarray data, knowledge of highly selective gene expression, as well as sequence homology to known gene families can provide convenient short cuts for better understanding of disease and unravel new information about pathways and cellular functions.

The genome wide data analysis typically requires semantic integration and constant updating of diverse types of annotation data, as these databases are not only in different formats but are also rapidly evolving, leading to significant informatics efforts.

The Function Express gene anno-

tation server addresses these issues by combining management and integration of complex microarray data and distinct biological and clinical data types. It provides an enriched collection of functional information about selected genes drawn from various public domain databases for facilitating microarray data interpretation. The analysis tools integrated in Function Express facilitate analysis and visualization of the various data sets to expedite discovery of biomarkers.

The Function Express also includes Gene Literature Network, which generates network of genes based on co-citation in Pubmed abstracts. It is tightly integrated with Function Express to enabling correlations with Gene Ontology, etc.

Function Express is a two-tiered client-server Graphical User Interface (GUI)-driven application. The platform-independent (UNIX, Windows, etc.) server brings gene annotation data from various public databases and uploads it into the warehouse. Client machines running Windows (95, 98, NT, 2000, XP) connect to, communi-

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Management of Data

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cate with, and transfer data to and from the server.

Web-based Portal for Microarrays

We have also developed and deployed web-based tools at the Washington University server, which allow investigators to download chip data along with selected annotations.

The investigator can also use this interface to query the database, and publish chips. The sophisticated authorization and authentication methods that are implemented allow the investigator to selectively share their data with colleagues.

Mutation Analysis Pipeline-Integrating the Sequence and Mutation Data

The goal of a Microarray experiment is to screen interesting genes in patients' clinical samples by studying the genome-wide expression levels. These interesting genes are then actually sequenced using the same samples that were used for microarray experiments. These sequences are then stored

in the central database.

The Mutation Analysis Pipeline facilitates localizing mutations on the gene sequences from the clinical samples by comparison with reference sequence and verification with dbSNP database. The application pipeline helps the investigator right from primer design to the visual comparison of same genes from multiple samples or multiple genes from the same sample.

LIMS for Proteomics

Success of a Proteomics laboratory depends on rapid analysis by optimizing throughput, managing data and improving quality.

Our LIMS for Proteomics is a complete system that integrates and automates sample handling, sample analysis, role and resource management and integration of third-party tools for gel image and protein expression analyses.

LIMS for Proteomics integrates the workflow from initial sample characterization through gel analysis to protein identification. From a single central screen, the investigator can design experiments, set parameters,

generate protocols and workflows. The bar-coding capability simplifies tracking and processing of multiple samples for multiple projects. Tracking of experiments is simplified through the hierarchical relationship between samples, gels, and spots.

Laboratory resources can be managed effectively through LIMS interface by assigning multiple roles to one user or one role to multiple users with secure access to all or part of the system. Auto forwarding of completed task, auto initiation of new task and visual indicators for incomplete tasks automate workflow.

The most powerful feature of LIMS for Proteomics is its ability to interface with third party tools that enables it to capture information from gel reader and display results in a gel viewer. For instance, it maps Cartesian coordinates of the significant spots selected in 2-D Gel electrophoresis image (image1) generated by Ettan™ DIGE system (Amersham Biosciences) with the corresponding spots in the scanned image (image2) of the fixed gel generated by the ProPic™ software (Genomic Solutions), which is in a different orientation. The spot-list generated from image1 is transformed so that the coordinates reflect the same spots in image2. This transformed list is used by a robotic arm for precise cutting and picking of the spot material for further analysis (MS).

To maximize the opportunity for discovery, the built-in protein identification viewer integrates spots on the gel image with the Mascot search results. Clicking on the spot generates a consolidated, succinct report from multiple MS jobs on the spot; different color labels are used for each job. This allows protein identifications to be related to the experimental workflow. All the data are viewed in one fully integrated system. Reports can be generated at any stage to track progress of experiments or review final results.

Advantage of Approach

The data warehousing based solution has the advantage of having all the data in one place, which is transformed to match the desired queries.

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The queries are fast, and there is no dependence on individual data sources.

Data Integration Solutions for Sequencing Pipeline at MIT-Broad Institute

The MIT-Broad Institute for Genome Research is one of the largest genome centers in the world and has served as one of the flagship centers of the Human Genome Project. Today, the center houses a broad range of thriving research programs combining structural genomics, medical, population genetics, and clinical medicine.

The sequencing laboratory at the center produces over 50 billion high-quality nucleotide base calls per year, each of which has multiple pieces of information associated with it. The amounts of data produced by sequencing raise significant challenges for informatics resources. The existing operational OLTP (Online Transaction Processing) system (Production Database), which hosts the data generated by genome sequencing process, is a huge system with thousands of tables and terabytes of data. The production database is continuously updated and hence heavily loaded, as the sequencing center runs 24/7. The report generation and analysis queries put extra burden on the production database.

To resolve the reporting and integration issues at the sequencing center at the Broad Institute, we are building a data warehousing solution that will take the analysis load off the production database and facilitate complex analytical queries. The major challenges involved in implementing the desired solution were acquiring requisite domain knowledge, understanding the schema of the production database, understanding the reporting and analysis needs of the Institute, designing the warehouse schema and summaries for optimizing report generation, designing the ETL transformations, and designing the physical database. The Warehouse developed and deployed at the sequencing center includes Initiative Management and Lab Quality

Data Marts.

The Initiative Management Data Mart efficiently integrates the data related to the sequencing process (a small part of the production database), and is optimized for generating project management reports.

The Lab Quality Data Mart addresses the complex problem of associating the lab workflow information with the quality of the sequencing process. The lab workflow involves various phases, such as addition of reagents to the samples (DNA fragments) that are to be sequenced, transferring the samples from one plate to another, and processing of the samples at several decks (machines). Any defect or shortcoming in a workflow phase can lead to deterioration of the quality of sequenced samples. The data mart links the quality of samples to various factors of lab workflow such as materials, plates and decks involved in the sequencing process, and temperature/humidity of various phases of the workflow. The main purpose of the data mart is to allow users to identify and analyze the factor(s) that lead to drop/rise in the sequencing quality.

The data marts are built on Oracle 10g, and Cognos-Cubes are used for reporting and analysis. Oracle Streams is used in the extraction phase to identify the changes made in the OLTP databases and to copy the changes to a staging area. Oracle Streams can read archive logs of the OLTP database without affecting normal processing of the OLTP system, to efficiently detect the relevant inserts, updates and schema changes made to the tables in the OLTP system. Oracle Warehouse Builder (OWB) is used as the ETL (Extract-Transform-Load) tool to transform and load the staging production data to the data marts.

Conclusion

The widespread adoption of high throughput technologies and exponential increase in the volume of available data are challenges often cited in the integration of biological and clinical data. Although, modern data management technologies provide solutions that address data scale-up problems,

the intricacy of biological and pharmaceutical R & D data needs to be carefully considered in order to devise the correct integration solution.

For selecting the most optimum data integration methodology, we at Persistent Systems have thoroughly examined the requirements and complexity of data, in the case of both Washington University and Broad Institute.

While implementing solutions for the School of Medicine, Washington University in St Louis, the highly specific scientific questions of relationships between the expressions values for genes and the experiment and the biological context were taken into consideration. Solutions were devised such that the data model created explicit representation of the relationships in the system, allowing formulation of queries that answered the researchers' questions. A complete research workflow often requires that the computational tools be able to process and display the integrated data in a succinct manner. The computational tools developed and deployed for Washington University help capture, disseminate, share, query and visualize post-genomic data. Similarly, while implementing data marts for MIT-Broad Institute sequencing pipeline, issues of huge volume of data, intricate workflow and complex query report requirements were taken into consideration. The value added by our solution provides a compelling argument in terms of the time and effort saved in accessing multiple disparate data sources and aiding decision support system.

Dr. Raghunath A. Mashelkar, Director General of the Council of Scientific and Industrial Research has stated "Rapid paradigm shifts that are taking place in the world, as it moves from super-power bipolarity to multipolarity, as industrial capitalism gives way to green capitalism and digital capitalism, as information technology creates netizens out of citizens, as the nations move from 'independence' to 'interdependence', as national bound-

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Tailoring Chemistry

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in a matter of seconds.

I did not ask Jordi about the challenges he faced in synthesizing the large number of chromatographic (GPC) columns his company now markets to major pharmaceutical and biochemical companies. Jordi makes GPC packings from 100% polydivinyl benzene (DVB) to assure compatibility with high temperatures, high pressures and the widest range of solvents. A single Jordi GPC column replaces several fragile PS-DVB columns and expands the range of solvents available for solving several polymer analysis problems. The analytical chemist is thus able to use one single Jordi GPC column with toluene, THF, methanol, hexane, HFIP, acetone, Freon, or 5% water in THF.

Many of Jordi's clients in the pharmaceutical and biotech industry synthesize or use a great number of polymer-based products or additives. When it comes to analytical methods for polymers, Jordi and his staff specialize in dealing with these kinds of polymer-related problems. That is primarily due to Jordi's, and his staff's, extensive chemical background in polymer chemistry; and in particular, their synthesis work. On his company's website, (www.jordiassoc.com), Jordi provides a complete database of all the procedures his laboratory uses in its analytical work.

I was wondering whether that means Jordi has a *carte blanche* from his clients in what analysis his company should do, so I asked him whether that is the situation.

"This is not the case," Jordi responded. "In Polymeric Analytical Chemistry, analysis could get to be expensive. Therefore, knowledgeable clients have to be selective." Jordi's laboratory provides the following services: Gel Permeation Chromatography (GPC), High Temperature Gel Permeation Chromatography, Polymer Deformation, Liquid Chromatography (LC) (method development), Liquid Chromatography (LC) (most standard methods), Gas Chromatography (GC)

(method development), Gas Chromatography (GC) (most standard methods), Differential Scanning Calorimetry (DSC), Titimetry, Infrared Spectroscopy (IR), Attenuated Total Reflectance Spectroscopy (ATR), Ultra-Violet - Visible - Spectroscopy (UV/Vis), Thermogravimetric Analysis (TGA), and Thermal Mechanical Analysis (TMA), as well as LCMS, GC/MS and desorption GC/MS testing.

Jordi is aware that costs could be a limitation and could discourage his client when he sees the price tag. Therefore, in general, he encourages his clients to do their own analysis in house and use the outsourcing option when it is more cost-effective. And in fact, his staff works with the clients to do just that.

Typically, Jordi's clients know that a subset of the total analytical work they need requires sophisticated equipment, software, and manpower they do not have at their disposal. Especially during the research phase of the project, they would not try to justify any major capital outlays for extensive analytical work rather than for the synthetic work. Besides, the qualified and experienced manpower for complicated analysis is just not available. Those clients know the type of analysis they want conducted and, therefore, they are able to define the analytical task they want (in collaboration with Jordi's staff as needed). Why would a chemist who has just developed a compound let an outside expert do an analysis rather than do it in his own laboratory?

"They would like to know all the compounds and by-products of a newly synthesized compound. There are bound to be surprises, both positive and negative, that could be revealed in a more sophisticated laboratory such as Jordi's," Jordi commented. As for security concerns, Jordi signs non-compete agreements to protect the client.

According to Jordi, his company's analysis is more accurate and comprehensive than that provided by a chemist who has just synthesized a new compound and has to conserve his cash for other purposes. Not only is Jordi's laboratory better equipped and

staffed than those of most of his clients, but it is also independent. After all, an outside laboratory such as Jordi's has no vested interest in the analytical findings. Some clients value an independent analysis in the case of a new compound, particularly where the client has to deal with investors, government agencies, and entrepreneurs.

Jordi added, "There is also the issue of reproducibility. In science, data should be reproducible by more than one individual. When our laboratory can duplicate the results from another organization, we then have confirmation of the overall data accuracy."

In production, in particular, the relatively stable variability of the data from one batch of the product to another shows how reliable the manufacturing process is, as well as how stable the product is under various conditions.

Another group of clients are the law firms who would like to base their cases on findings that are made through independent analysis. For example, independent laboratories identified the increasing nicotine levels in cigarettes over the years. Other cases include an identification of foreign poisonous contaminants (in minute quantities) contained in foods, drinks, or drugs sold to consumers.

Where does the FDA or the EPA come in? Both agencies are interested in independent reproducibility, and expect companies to use an independent laboratory, such as Jordi's, that is open for inspection and audit, as well as the analysis be conducted in accordance with recognized standards, such as the ASTM. Jordi's laboratory is certified by the FDA or EPA to perform certain analyses.

In reality, Jordi himself acknowledged that his staff chooses to outsource part of the effort to various sources with whom he has established

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Tailoring Chemistry

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some working relationships rather than try to duplicate the expertise acquired by some of the laboratories. In fact, Jordi does provide the following services through outside affiliates:

- a. Elemental X-Ray Analysis including: Elemental Spectroscopy for Chemical Analysis (ESCA), Energy Dispersive Spectroscopy (EDS) Scanning Electron Microscopy (SEM) Fluorescence SP ARK Source Mass Spectroscopy, Inductively Coupled Plasma Emission Spectroscopy (ICP), Atomic Absorption Spectroscopy (AA).
- b. Organic Structural Characterization: Nuclear Magnetic Resonance Spectroscopy (NMR), including proton and carbon 13.

In those cases where Jordi's laboratory chooses to outsource, Jordi's staff is involved in supervising the total process, which includes the preparation of a report.

In most applications each client who decides to outsource the analytical chemistry effort to Jordi's laboratory has a unique problem. It is the client's responsibility to define the problem. In response, Jordi's staff proposes a specific analytical solution to the client in terms of priorities, timelines, costs, and expectations, thus giving the client a choice on how to proceed with the overall analytical effort. At some point, there is a meeting of the minds on what analytical tasks will be performed by which laboratory and on which timeline. Tailoring the analytical chemistry effort to deal with the specific chemistry problem will ultimately assure the client that the information needed will be acquired and made available at the appropriate time of the project and at optimum costs. ◇

Historical Notes

Homer F. Priest

Homer F. Priest retired former Director of the Materials Research Laboratory, U.S. Army Materials Research Agency, Watertown Arsenal, died March 12, 2004 at the age of 88. Born June 14, 1916 in Nelson, NH, Priest received his bachelor's degree in chemistry from the University of New Hampshire in 1938 and his master's degree from Williams College in 1940. On November 28, 1941, he married Grace L. Ernst, also a chemist. He was an instructor in chemistry at Columbia University from 1940-1941 while working on his doctorate with Professor Harold Urey. While at Columbia he and his wife were enlisted to work on the Manhattan project. From 1941-44 he was head of the Chemistry Division and a Section leader at the K-25 Gaseous Diffusion Plant, Oak Ridge, Tennessee, where he and his wife studied uranium hexafluoride chemistry and performed materials research to develop barriers for the separation of uranium isotopes in the gaseous diffusion process.

From 1944-1946, he was employed as a chemist by Carbide and Carbon Chemical Corporation, at Oak Ridge, Tennessee. In 1946, he was named Director of Research. From 1948-1950, Priest was appointed as Technical Advisor to the Chief of the Technical Command, Decontamination Branch, Radiological Warfare Division, U.S. Army Chemical Center, Edgewood Arsenal, Maryland.

He received his Ph.D. in Inorganic Chemistry from Massachusetts Institute of Technology in 1948 under Professor W. C. Schumb. After receiving his Ph. D., he was a consultant in the

materials field. From 1951-1954 Priest served as Assistant Group leader, Solid State Transistor Group, Lincoln Laboratory, Massachusetts Institute of Technology. While at Lincoln Laboratory he held a concurrent position as Executive Assistant to the President, High Voltage Engineering Corporation, from 1950-1951. He then left Lincoln Laboratory to join the Solid State Research Group at Baird Associates and remained there until 1957.

Priest served as a Supervisory Physical Chemist, Materials Research Laboratory, Ordnance Materials Research Office, U.S. Army Watertown Arsenal from 1957-1963. In 1963 Priest was appointed Director, Materials Research Laboratory, U.S. Army Materials Research Agency, Watertown, Massachusetts. Priest's last position was Chief, Materials Science Division, U.S. Army Materials and Mechanics Research Center, Watertown, Massachusetts. He retired from this position in 1980.

Dr. Priest received an Honorary Doctor of Science Degree from the University of New Hampshire in May of 1968 in honor of his contributions to the Manhattan Project and the development of techniques for growing single crystals of semiconductor materials.

He was an avid birder and bird photographer and spent most of his winter vacations in Florida observing and photographing in the everglades. He enjoyed working outdoors in his garden and yard. He was a lifelong member of the Massachusetts Audubon Society, the National Audubon Society, and the National Wildlife Federation.

He is survived by his wife of 63 years, Grace Priest. He was an emeritus member of the American Chemical Society with 65 years of membership.

Submitted by Dr. John R. Hobbs

Historical Notes is an ongoing series of short biographies of recently deceased chemists and chemical engineers whose deaths have been reported to us during the past year. We thank members of the Northeastern Section who have sent us obituary notices appearing in community newspapers we do not see. ◇

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aries become notional, and as the concept of global citizenship gets evolved, will see a world full of new paradigms and new paradoxes. There is no doubt that the rapid advance of science and technology will directly fuel many of these. The Indian pharmaceutical and IT sectors, in particular, the contract R & D organizations have seen a dramatic change in their capabilities and sophistication. International pharmaceutical companies should now be ideally poised to seek collaborations to bring innovative drugs to the consumers at an affordable price."

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Brandeis Univ., Edison Lecks Bldg.,
Gerstengang 122, 3:30 pm

Prof. David Eisenberg (UCLA)
(The Frank H. Westheimer Prize Medal.)
Harvard Univ., Pfizer Lecture Hall,
12 Oxford St., 4:15 pm

Prof. David Walt (Dept. of Chem., Tufts Univ.)
"Array-based Biosensing: DNA to Cell Arrays"
Tufts Univ. Chemical and Biological Engineering Seminar Series,
Science and Technology Center, Room 136,
4 Colby St., Medford, 12:00 m

Dec 8

Prof. Clemens Richert (Universität Karlsruhe)
"Chemical Primer Extension"
Tufts Univ., Pearson Chemistry Building,
62 Talbot Ave., Medford,
Room P-106, 4:30 pm

Dec 12

Prof. Joanne Stubbe (MIT)
"Ribonucleotide Reductases: Something for Everyone"
Brandeis Univ., Edison Lecks Bldg.,
Gerstengang 122, 3:30 pm

Notices for the Nucleus Calendar should be sent to:

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