SouthEast Chapter Laboratory Robotics Interest Group

Automation for the Chemistry Laboratory
An Invited Speaker Proposal for SERMACS

Prepared By: David Smith
Date of Publication: October, 20, 2003

Automation for the Chemistry Laboratory

Symposium Overview

The introduction of automation into the chemistry laboratory has played a key role in the increase of chemist's productivity. Technological advances over the past 15 years in such areas as Combinatorial Chemistry, High Throughput Purification, and Microfluidics has increased the number of molecules made and analyzed from 10-100's of compounds per chemist per year to 100,000's of compounds per chemists per year. Whether it is the use of liquid handlers for pipetting reagents, robotic arms moving plates, or LIMS systems tracking molecules and their related data, the chemist has at their disposal the tools and process to deliver more molecules with a greater confidence level in structural validity than at any time in the past.

The SouthEast Chapter of the Laboratory Robotics Interest Group proposes an invited speaker siminar focuses on the use of automation techniques in the chemistry lab. We propose that the invited speakers cover the topics of synthesis, macro and micro scale, purification and detection, and computing. The speakers will provide either a retrospective of their domain and a vision of the future or progress in their research.

Proposed Speaker List

H. Mario Geysen

- Alfred Burger Professor, University of Virginia
- B. Sc. Chemistry, University of Melbourne, Australia.
- M. Sc. Science (Chemical engineering), University College London, UK.
- Dip. Biochemical Engineering, University College London, UK.
- Ph. D. Microbiology, University of Melbourne, Australia

Email:geysen@virginia.edu

Combinatorial Sciences

Principle Research Interests

Combinatorial chemistry is best described as the intersection of many disciplines namely, chemistry, robotics, instrumentation, computer science, and engineering. It focuses on the use of very large numbers, either of the chemical entities themselves or of the number of trials (experiments), carried out in parallel to answer questions faster and more comprehensively than can be achieved by the more conventional sequential experimentation protocols. Another way of looking at combinatorial techniques is to think of a complex problem as a very large search space of all possible solutions, and where experimentation is carried out to generate many of these solutions with an adequate coverage of this space to rapidly determine an acceptable solution to the designated problem. The combinatorial procedure can readily be broken down into a number of well-defined steps, namely:

· Analysis of the problem and the definition of the appropriate search space.
· Design of the experimental protocol for the generation of candidate solutions.

Automation for the Chemistry Laboratory

· Use of robotics to carry out the required number of synthetic steps.
· Measurement (assay) of each outcome (compound/protocol) in terms of the problem at hand.
· Analysis of both the positive and negative data obtained, to gain the greatest insight into the properties and or characteristics of successful solutions to the problem.

In recent years combinatorial techniques are being applied to chemistry related endeavors other than to its original application, that of drug discovery. My research interests are centered on the demonstration and development of technologies applicable to any problem with a numerically large solution space.

Gary Kramer (http://www.cstl.nist.gov/nist839/839.04/kramer.html)

Gary Kramer received his Ph.D. from Purdue University in organic chemistry working with Professor H.C. Brown on the synthesis and reactions of allylic organoboranes. He joined Purdue's Chemistry Instrumentation Facility, where he designed analytical instruments and instrument interfaces, consulted on measurement problems, and co-directed a project to automate the way organic synthesis development is carried out in the laboratory for which he received a Pioneer in Laboratory Robotics award in 1985. In 1990, he joined the National Institute of Standards and Technology and served as Project Manager of the Consortium on Automated Analytical Laboratory Systems (CAALS), a U.S. industry/Government joint venture to foster the development of laboratory automation for analytical chemistry. In 1995, he was appointed Leader of the Chemical Sensing and Automation Technology Group, which was later renamed the Molecular Spectroscopy and Microfluidic Methods Group. In 1998, he received the Association for Laboratory Automation Achievement Award. Currently, in addition to his instrumentation and laboratory automation activities, he is working to develop standards for luminescence measurements and a markup language for spectroscopy result data interchange and archiving. He serves as a member of the NCCLS Area Committee on Automation and Informatics and chairs ASTM Subcommittee E13.15 on Analytical Data Management.

Contact:
Molecular Spectrometry and Microfluidic Methods Group
Analytical Chemistry Division
National Institute of Standards and Technology
100 Bureau Drive
Mail Stop 8394
Gaithersburg, MD 20899-8394
phone: 301/975-4132
fax: 301/977-0587
mailto:gary.kramer@nist.gov

Todd L. Graybill, Ph.D.

Dr. Graybill is currently a High-Throughput Chemistry team leader at GlaxoSmithKline, Collegeville PA. His team's focus includes identification of tractable medicinal chemistry starting points following high-throughput screening campaigns, use of parallel and iterative synthesis techniques for rapid property optimization of these hits (Hit to Lead), and use of automation for chemistry. Dr. Graybill also contributed to the design and current exploitation of a newly constructed automation facility at GSK.
Prior to his current responsibilities, Dr. Graybill held medicinal chemistry positions at 3-Dimensional Pharmaceuticals (Exton, PA) and Sterling Winthrop (Collegeville, PA) were his efforts focused on the combinatorial and rational design of orally-bioavailable peptidomimetic inhibitors of both serine and cysteine proteases. Dr. Graybill received his Ph.D. degree in Organic Chemistry from The Johns Hopkins University in 1990.

Contact:
GlaxoSmithKline
Discovery Research - High Throughput Chemistry
Mailcode UP12-205
1250 S. Collegeville Rd.
Collegeville, PA 19426
USA
Tel: 1-610-917-5870
Fax: 1-610-917-4206
e-mail: Todd_L_Graybill@gsk.com

Albert Van Den Berg

Albert van den Berg received his M.Sc. degree in Technical Physics at the University of Twente (Ir) in 1983 and made a Ph.D. degree in Technical Sciences at the same University in 1988 with prof. D.N. Reinhoudt and prof. P. Bergveld. He then worked as Project leader at the Swiss Center of Microelectronics (CSEM), Research scientist and project manager at the University of Neuchâtel (prof. N.F. de Rooij) and Research coordinator at the MESA Research Institute of the University of Twente for the research orientation Micro Total Analysis Systems (μTAS). He is member of numerous scientific organizations and committees (NanoTech, μTAS, ESSDERC, Eurosensor, MEMS, Gordon Research Conference, IMRET, Micromachine Symposium, Medtronic, Sentron CMT BV, NEXUS) and author of over 70 reviewed articles, several contributions to international textbooks and numerous posters on international conferences and meetings. He has 6 patents. Since 1998 he is Program director at the MESA+ Research Institute of the University of Twente (NL) for the research orientation Micro Chemical Systems (MiCS). 1998 he has been pointed as professor "Miniaturised (Bio)Chemical Analysis

Systems" and 2002 as professor/group leader "Sensorsystems for biomedical and environmental applications".

The Technology Foundation STW has awarded prof.dr.ir. Albert van den Berg and prof.dr. Cock Lodder the Simon Stevin Masterhood. This is the highest Dutch award for technical-scientific research.

Contact:
Prof.dr.ir. A. van den Berg
University of Twente
Faculty of Electrical Engineering
Laboratory of Biosensors
Micro Chemical Systems
P.O.Box 217
7500 AE Enschede
The Netherlands
Tel : +31 53 489 2760
Fax : +31 53 489 2287
A.vandenBerg@el.utwente.nl

Dr Paul Watts
BSc, PhD
email: p.watts@hull.ac.uk
Tele: +44 (0)1482 465471
Fax: +44 (0)1482 466416

Research

Organic chemistry and electrosynthesis in micro reactors
On-chip analysis of reaction mixtures

Career Resumé

1992-95	BSc in Chemistry, Department of Chemistry. University of Bristol
1995-99	PhD in Bioorganic Chemistry Department of Chemistry, University of Bristol

2000-2002	Postdoctoral research associate working on organic synthesis in microreactors Department of Chemistry, University of Hull
2002-	Lecturer in Analytical Science Department of Chemistry, University of Hull