

IPUS

**BIOINFORMATICS SYMPOSIUM OF THE ANALYTICAL DIVISION OF THE
AMERICAN CHEMICAL SOCIETY MEETING**

Final Technical Report from 03/15/2000 to 03/14/2001

Robert T. Kennedy

**University of Michigan
Ann Arbor, MI 48109**

August 2002

Prepared by the U.S. DEPARTMENT OF ENERGY

Award Number DE-FG02-00ER62938

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

On March 28, 2000 the Bioinformatics Symposium was held at the ACS National Meeting in San Francisco. In this symposium we brought together analytical chemists who were developing novel techniques to generate information on genomes, proteomes, or cells with informatics experts who were developing data mining and modeling algorithms and software. The goal of the symposium was to highlight the role and opportunity for analytical chemistry research in the informatics revolution that is changing the face of biological research.

The following presentations were given:

- "Trends, opportunities, and challenges in bioinformatics" by J.C. Wooley (UC-San Diego)
- "Integrative Bioinformatics: bridging the chasm between genomics and cell biology" by R.D. Phair (Bioinformatics, Inc.)
- "Profiling signal-transduction networks in single mammalian cells" by N.L. Allbritton (UC-Irvine)
- "Integrated software tools for functional genomics" by T. Ferrin
- "Bioinformatics in the chemical process industry" by L.D. Rothman (Dow)
- "Past, present, and future of the protein data bank as an enabling resource" by H.M. Berman (Rutgers U.)
- "Analyzing genetic variations by mass spectrometry" by L.M. Smith (U. Wisconsin)
- "Signal transduction in insulin secretion: An opportunity for bioinformatics" by R.T. Kennedy (U. Florida)
- "Integrated view of bioinformatics for both genomics and proteomics" by W.S. Hancock (ThermoFinnigan)

Several themes emerged from this series of talks. The tools for genomics and proteomics are highly generalized and quite sophisticated for analyzing sequence data. Such data/data analysis tools are rapidly becoming an indispensable tool for the pharmaceutical and biotechnology industry. While DNA sequencing technology is now quite robust and well-developed, analysis of genetic variations, proteomes, and cellular biochemistry still requires considerable research to generate information at the level need for a bioinformatics approach. Cellular data requires both temporal and spatial resolution to be of use.

We estimate that over 200 people were in attendance for each talk. Based on the strong attendance throughout the day and the extensive discussions that resulted after each talk, the symposium was considered highly successful.

219th BOOK OF ABSTRACTS



SAN FRANCISCO

ACS National Meeting
March 26-30, 2000

ABSTRACTS OF PAPERS

Part 1

219th ACS National Meeting
0-8412-3731-X

American Chemical Society

San Francisco, CA

March 26-30, 2000

American Chemical Society
DIVISION OF ANALYTICAL CHEMISTRY
ABSTRACTS

219th ACS National Meeting

San Francisco, CA
March 26-30, 2000

T. R. Williams, Program Chair

SUNDAY AFTERNOON

• **Chemical Microscopy**

W. C. McCrone, Presiding; D. A. Stoney, Organizer

Papers 1 - 4

• **Microchip-Based Chemical Separations**

J. M. Ramsey, Organizer, Presiding

Papers 5 - 10

SUNDAY EVENING

• **General Papers**

T. R. Williams, Presiding

Papers 11 - 155

• **I. M. Kolthoff Awards**

S. Daunert, Organizer, Presiding

Papers 156 - 165

MONDAY MORNING

• **ACS Awards in Analytical Chemistry**

T. R. Williams, Presiding

Papers 166 - 167

• **Biotechnology and the Analytical Chemist: Roles and Career Opportunities**

T. Babarakis, Organizer, Presiding

MONDAY AFTERNOON

• **Microchip-Based Chemical Separations**

J. M. Ramsey, Organizer; S. C. Jacobson, Presiding

Papers 168 - 173

• **Chromatography in the 21st Century**

R. L. Wixom, Organizer

Papers 174 - 179

TUESDAY MORNING

• **Bioinformatics**

R. F. Hirsch, Organizer; H. Blount, Presiding

Papers 180 - 183

TUESDAY AFTERNOON

• **Bioinformatics**

R. Hirsch, Organizer; H. Blount, Presiding

Papers 184 - 188

• **Material Science: New Products, New Challenges**

J. Mitchell, Presiding

Papers 189 - 194

• **Analytical Problems of the 21st Century**

T. R. Williams, Organizer, Presiding

Papers 195 - 199

WEDNESDAY MORNING

• **Immunochemical Methods for the 21st Century: Immunochemistry Summit**

J. M. Van Emon, Organizer, Presiding

Papers 200 - 207

disposability obviates carryover and contamination problems. Applications in drug screening and genetic analysis, where the use of electrophoretic separations is a key to effective performance, will be described.

171. HIGH-ASPECT RATIO MICROMACHINING IN PLASTICS: A LOGICAL CHOICE FOR THE FABRICATION OF DNA ANALYSIS DEVICES. *Stephen A. Soper, Kevin Kelly, Robin McCarley, Sean Ford, Shize Qi, Scott McWhorter, Gloria Thomas, Suzanne Lassiter, Alyssa Henry, and Yun Wang. Louisiana State University, Baton Rouge, LA 70803, steve.soper@chemserv.chem.lsu.edu*

LIGA micro-machining can be used to produce mold inserts with very high aspect ratios to fabricate microstructures (HARMS) with small dimensions and relatively large heights (or depths). For example, using LIGA, narrow channels (~10-20 mm) with large depths (50-100 mm) can easily be machined to perform fluidic-type functions. In addition, these HARM inserts can be used to produce microchips in various types of plastics using either hot embossing or injection molding. We have initiated work on fabricating microchips in polymethylmethacrylate (PMMA) for electrophoresis-based applications specifically targeted toward analyzing DNAs. Due to the fact that deep channels with narrow widths can be fabricated, fluidic interconnects to the chip can be made using conventional capillary tubes with minimal unswept volumes for convenient sampling from titer wells containing sequencing or genetic samples. In our presentation, we will discuss the fabrication of PMMA microchips using LIGA processing, the assembly of PMMA devices and also, material properties of PMMA. We will also discuss robust surface modification procedures in PMMA to alter the electroosmotic properties of the material. Finally, we will discuss results using multi-channel devices for high throughput sequencing and/or genetic analyses.

172. POLYMERIC MICROFLUIDIC SYSTEMS WITH INTEGRATED ELECTROCHEMICAL DETECTION FOR DNA ANALYSIS. *Werner G. Kuhr, Sara Brazill, C Brandon Davis, Binayak Roy, and Joan Stuart. Department of Chemistry, University of California, Riverside, CA 92521, fax: 909-787-4713, werner.kuhr@ucr.edu*

A PDMS microfluidic chip has been developed which allows for the direct detection of several distinct DNA targets present in a sample. Electrochemical detection of DNA is accomplished with integrated electrodes in very small volumes. The DNA sample can be labelled with an electroactive tag and separated in a sieving buffer with capillary electrophoresis for DNA sequencing. Alternatively, DNA hybridization probes can be attached in the microchannels on the chip via a biotin/avidin linkage. Following hybridization of the target, an alkaline buffer is introduced to the channel to dehybridize the double-stranded DNA and flush the target downstream to a copper electrode. The dehybridized DNA is then detected electrochemically. Integrating the detector and the sensing probes on the microfluidic chip allows for an inexpensive and easily fabricated biosensor device for the precise recognition and subsequent detection of a specific complimentary DNA target for diagnosis and genetic screening.

173. MICROSYSTEMS FOR CHEMICAL ANALYSIS. *Scott D. Collins, Carlos Gonzalez, Kin Yan, and Rosemary L. Smith. Department of Electrical Engineering / MicroInstruments and Systems Laboratory, University of California, One Shields Ave, Davis, CA 95616, fax: 530-758-8103, collins@ece.ucdavis.edu*

Presented here is a basic overview of the current state of microsystem development for chemical analysis. More specifically, the overview highlights three specific microsystems recently developed at MISEL, and their fabrication, function, characterization, and limitations to chemical analysis will be discussed. The three microsystems include: 1). A surface plasmon resonance microinstrument (SPR). The SPR not only provides generic detection for HPLC or affinity chromatography, but provides simultaneous chemical analysis of the effluent. The small size of the detector, 1cm x 2cm x 0.5cm, also allows use as a stand-alone sensor for remote or biologically hostile areas. 2). A miniature Fourier Transform Spectrometer (FTS) predicated on the Michelson interferometric with a resolution of <0.1cm⁻¹. Because of its small size, 10cm x 5cm x 1.5cm, the FTS is extremely portable and may be used as a automated sensor to monitor virtually any desired set of preprogrammed chemical signatures through the use of standard pattern recognition algorithms or appended to the output of any chemical separation system for analysis. 3). A modular electro-

phoretic separation microsystem for the massively parallel separation and analysis of combinatorial chemistry products. (<http://ece.ucdavis.edu/misl/Homepage.htm>).

174. HPLC COLUMN TECHNOLOGIES IN THE NEW MILLENNIUM. *Ronald Majors, AL*
Abstract text not available.

175. PROSPECTS IN CAPILLARY-ELECTRAL CHROMATOGRAPHY. *Zsabag Horvath, B/A, MO*
Abstract text not available.

176. SEPARATING MICROBES IN THE MANNER OF MOLECULES. *Daniel Armstrong, University of Missouri, Rolla, MO 65401, fax: 573-341-6033*
Abstract text not available.

177. FAST SOLVATING GAS CHROMATOGRAPHY FOR CHIRAL SEPARATION. *Milton Lee, Analytical Chemistry, University of Utah, UT, fax: (801) 378-5474, milton_lee@byu.edu*
Abstract text not available.

178. PROGRESS AND PROSPECTS FOR SEPARATION OF POLYMER SYSTEMS. *R. Tijssen, University of Amsterdam Netherlands*
Abstract text not available

179. STRUCTURE IN THE DEVELOPMENT OF AFFINITY CHROMATOGRAPHY. *Robert Wixom, University of Missouri, M121 Med. Sci. Building, Columbia, MO 65212*
Abstract text not available.

180. TRENDS, OPPORTUNITIES, AND CHALLENGES IN BIOINFORMATICS. *John C. Wooley, Associate Vice Chancellor for Research, University of California, San Diego Supercomputer Center, 9500 Gilman Drive, MC 0505, La Jolla, CA 92093-0505, fax: 858-822-0948, jwooley@ucsd.edu*

In the "sequenced genomes era," often called beyond the genome, extraordinary challenges and opportunities await in determining the chemistry of protein-protein interactions and cellular networks, the architecture of supramolecular structures, and many other research areas necessary to describe the complexity of living systems. Data intensive computing environments and the need to use computer tools to turn biological data into knowledge—one definition of bioinformatics—will underpin future biochemical and biophysical investigations that will begin with the knowledge of the genome sequence for all major organisms used in molecular research, but will need to uncover the chemical mechanisms by which the gene products function. The success of molecular biology in understanding single-gene diseases is "a hard act to follow" as we move toward what appear to more typical multigene traits. What will such data look like? Biological data are characterized by hierarchical complexity and uniqueness (that is, the data are not reducible by symmetric or temporal considerations); this contrasts with the huge but highly redundant data sets from meteorology and astronomy. Due to the nature of the research and of living systems themselves, the database efforts as a whole can not be effectively

coordinated. As a consequence, biological data is also stored, managed, and manipulated as—in effect—a “cottage industry” with no standards of nomenclature or representation routinely used. Providing tools that allow individual users not just to access but to compute on multiple data resources is one of the major challenges of bioinformatics. Today, information science and computational science provide critical tools for biochemistry, from focusing experimental studies to providing discovery tools for insight that otherwise could not be obtained.

181.

INTEGRATIVE BIOINFORMATICS: BRIDGING THE CHASM BETWEEN GENOMICS AND CELL BIOLOGY. *Robert D. Phair, Bioinformatics Services, 12114 Gateway Drive, Rockville, MD 20854, fax: 413-487-5098 rphair@bioinformatics-services.com*

Twenty-first century analytical chemistry will produce a tidal wave of experimental data that will swamp our human abilities to comprehend and integrate information. These enormous databases will, however, also contain hidden keys to complex diseases. Bioinformatics aims to provide computational tools for extracting this vital information. Beginning with an overview of bioinformatics from the perspective of 30 years as a bench/computational biologist, I will define integrative bioinformatics as a set of tools for testing modern biology's cellular signaling diagrams by translating them into computer models consisting of large systems of differential equations, and then applying the experimental protocol. In this way we can know with precision what the diagram predicts, and we can compare these predictions to the experimental time-course data. This comparison, with the help of modern optimization techniques, provides a powerful quantitative test of the hypothesis represented by the signaling diagram. My examples will be from cell biology.

182.

PROFILING SIGNAL-TRANSDUCTION NETWORKS IN SINGLE MAMMALIAN CELLS. *Nancy L. Allbritton, Gavin D. Meredith, Christopher E. Sims, and Joseph S. Soughayer. Dept. of Physiology & Biophysics, University of California, Irvine, D380, Medical Sciences I, Center for Biomedical Engineering, Irvine, CA 92697, fax: 949-824-8540, niall@uci.edu*

A central goal of genomics and proteomics is to catalog the biological molecules present in different organisms and cell types under various conditions. A greater challenge for accurate and comprehensive characterization, however, lies in determining the activities and functional relationships of the biological molecules, particularly the enzymes, as they occur within the complex cellular networks that comprise biological systems. To accomplish this task, new technologies must be developed to measure multiple chemical species within intact intracellular networks. We have demonstrated a new method for the simultaneous measurement of the activation of key regulatory enzymes in a single cell. This assay strategy should be broadly applicable to single-cell measurements of a broad range of enzymes, including kinases, phosphatases, proteases, and nucleases. New bioinformatic tools will need to be developed to describe and predict outputs from the signal transduction networks comprised of these enzymes. Multidisciplinary approaches will be required to unravel the complex signaling networks controlling cellular responses.

183.

INTEGRATED SOFTWARE TOOLS FOR FUNCTIONAL GENOMICS. *Thomas Ferrin, Patricia Babbitt, Conrad Huang, and Teri Klein. Computer Graphics Laboratory, University of California, San Francisco, CA 94143-0446, fax: 415-502-1755, tef@cgl.ucsf.edu*

The successes of the genome projects have largely solved the problems of mapping, sequencing and annotation to produce the enormous volumes of information currently available. Now, in the post-genomic era, the tasks are both more difficult and diverse, requiring new theoretical constructs and technologies for turning this information into knowledge. For example, we currently have no unified theory for the prediction of function from sequence or structure. An effective solution to this problem requires the ability to compute with function, which is currently not possible. In recent research work at UCSF, we have begun to address this issue through development of new computational

methods for integrating sequence and structural information to enable explicit mapping to function. This work includes designing, building, and integrating computational and visualization tools for constructing and manipulating protein superfamilies. This talk will describe some of these tools and how they might be extended to be useful for the entire genomic space.

184.

BIOINFORMATICS IN THE CHEMICAL-PROCESS INDUSTRY. *L. David Rothman, Dow Chemical Company, 1776 Building 2nd Floor, Midland, MI 48674, fax: 517-638-9707, ldrothman@dow.com*

Advances in analytical chemistry have enabled the production of massive amounts of gene and protein sequence and structure data. Analytical chemistry also provides a means to identify and measure metabolites to aid understanding organism metabolism. The chemical process industry has interest in sequence and metabolism data as a means to develop new products and raw materials. This presentation will discuss the interaction of analytical chemistry and computing science in the generation, management and interpretation of these data.

185.

PAST, PRESENT, AND FUTURE OF THE PROTEIN DATA BANK AS AN ENABLING RESOURCE. *Helen M. Berman¹, John Westbrook¹, Philip Bourne², Helge Weissig², Gary Gilliland³, and T. N. Bhat³. (1) Department of Chemistry, Rutgers University, 610 Taylor Road, Piscataway, NJ 08854, fax: 732-445-4320, berman@rcsb.rutgers.edu, (2) San Diego Supercomputer Center, University of California, 9500 Gilman Drive, La Jolla, CA 92093, (3) National Institute of Standards and Technology, Gaithersburg, MD 20899*

The Protein Data Bank began as a flat file archive for the storage of information on biological macromolecular structures. As the technology for determining the structures of molecules improved the number of structures increased, as did the demand for information about these structures. Thus, it became imperative to develop a system that allowed for high throughput data processing and versatile access to the primary and derived data. A description of the system that is currently in place will be given as well as examples of the type of research that the PDB has enabled. A vision for the future of the PDB resource and how it is expected to interact with new initiatives in structural bioinformatics will be described.

186.

ANALYZING GENETIC VARIATIONS BY MASS SPECTROMETRY. *Lloyd M. Smith, Department of Chemistry, University of Wisconsin-Madison, 1101 University Avenue, Madison, WI 53706-1396, fax: 608-265-6780, smith@chem.wisc.edu*

In the last decade two powerful new tools for the mass spectrometric analysis of biomolecules have been developed, Matrix-Assisted Laser Desorption Mass Spectrometry (MALDI-MS), and Electrospray Ionization Mass Spectrometry (ESI-MS). The power of these methods lies in their ability to produce and mass analyze intact gas phase ions from very large molecules such as proteins and nucleic acids. The speed, accuracy, and sensitivity of the technologies make them well-suited to address a number of problems in genetic analysis, including the analysis of DNA sequence, genetic variations, and gene expression. Results in these areas will be presented, including recent work in which single nucleotide polymorphisms (SNPs) in genomic DNA may be analyzed without need for a prior PCR amplification step.

187.

SIGNAL TRANSDUCTION IN INSULIN SECRETION: AN OPPORTUNITY FOR BIOINFORMATICS. *Robert T. Kennedy, Chemistry, University of Florida, P.O. Box 117200, Gainesville, FL 32611-7200, rt kenn@chem.ufl.edu*

Defects in insulin secretion are associated with Type II diabetes, therefore a greater understanding of the biochemical mechanisms underlying insulin secretion are of great significance. It is accepted that glucose metabolism by beta-cells of the pancreas is transduced into insulin secretion by a series of biochemical and biophysical events. In this talk, we describe how novel

microsensors, fluorescence microscopy, and gene-knockout technology have been used to unravel some of the chemical events involved in insulin secretion at the single cell level. It is demonstrated that multiple signal transduction pathways may interact resulting in a process that requires extensive use of bioinformatics to develop an appropriate model.

188.

INTEGRATED VIEW OF BIOINFORMATICS FOR BOTH GENOMICS AND PROTEOMICS. *William S. Hancock, Agilent Laboratories, 3500 Deer Creek Road, MS26U-6, Palo Alto, CA 94304-1126, fax: 650-857-2860, william_hancock@agilent.com*

The relationship of functional genomics to proteomics will be a key issue in the post-genome era. Functional genomics will be based on the study of the transcription/translation process and thus is a measure of the functionality of a given genome. The term proteome has been introduced to define the full complement of proteins in a cell and thus requires description of the localization, concentration and multi-subunit associations of each of these proteins. Another requirement is the definition of the post-translational modifications such as glycosylation, phosphorylation and sulfation as well as the incorporation of lipid components. These modifications often play a key role in the activity, localization and turnover of an individual protein species. Such measurements have become even more challenging with the recent revolution in sequencing of the human genome that will result in the discovery of several hundred novel protein sequences of unknown function. Thus the field of proteomics will require the development of a new set of analytical tools that allow the resolution and characterization of complex sets of protein mixtures in a high throughput manner. This presentation will describe the development of new instrumentation aimed at this challenge, such as high efficiency separations coupled with mass spectrometry. The presentation will also focus on strategies for integration of both genomic and proteomic data in the context of the biological system.

189.

CHARACTERIZATION OF MODERN AUTOMOTIVE FINISHES BY FOURIER-TRANSFORM MASS SPECTROMETRY. *William J. Simonsick, Jr, DuPont Performance Coatings, DuPont Marshall Research and Development Laboratory, Marshall R & D Laboratory, 3401 Grays Ferry Ave, Philadelphia, PA 19146, fax: 215-539-6087, william.j.simonsick@usa.dupont.com*

The chemistry of automotive coatings has undergone tremendous changes over the past twenty years in response to environmental pressures to reduce the volatile organic content (VOC) and an increase in consumer expectations for appearance and durability of the finish. Furthermore, the use of organic pigments is increasing in today's coatings due to environmental, health, and durability issues. Significant overlap now exists between the molecular weights of modern coating components and the mass range amenable to Fourier transform mass spectrometry (FTMS). One popular approach to lowering the VOC is the use of high solids (70%) low-molecular-weight (<5000 Daltons) enamels.¹ However, structural imperfections in the organic molecules used in high solids formulations have a more profound impact on final properties than do imperfections in their low solids high-molecular-weight predecessors, therefore sophisticated analytical techniques are required. For polymers, soft ionization methods using CO₂ laser desorption or electrospray ionization afford both the chain length distribution and the chemical composition at every chain length. Gel permeation chromatography can be coupled to FTMS through an electrospray ionization interface to characterize telechelic polymers.² Using quadrupole axialization and collisional cooling, high resolutions are possible for end group determinations. Tandem MS studies performed on polymer molecular ions provide information about the specific architecture and functionality location. Using CO₂ laser desorption molecular ions are furnished for organic pigments contained in cross-linked colorcoats.

190.

DETECTION AND CHARACTERIZATION OF INDIVIDUAL SUBMICRON PARTICLES BY LASER MASS SPECTROMETRY. *William D. Reents, Zhaozhu Ge, J. Eric Hower, Mark Morris, and Sanjay Patel. Bell Labs, Lucent Technologies, Murray Hill, NJ 07974*

Real-time detection and elemental characterization of particles using a single particle analyzer, the Particle Blaster, is described. This technique contrasts with

typical off-line elemental analyses provide results after a significant time lag, thus losing real time feedback or short term changes in particle characteristics. Ions are produced from individual particles by laser atomization/ionization and then analyzed with a time-of-flight mass spectrometer. The ion/mass signals provide information on the complete elemental composition of each particle as well as the particle's size. This technique has been applied to detection of particles in a semiconductor process tool under normal operating conditions (plasma on, 8 mTorr pressure) as well as preformed particles (silica, alumina, polystyrene) in aqueous solutions. Both major and minor elements are detected in each particle, typically to 100 ppm levels.

191.

MEASURING ADSORPTION AND MONOLAYER FORMATION AT LIQUID INTERFACES BY VIBRATIONAL SUM-FREQUENCY SPECTROSCOPY. *Geraldine L. Richmond, Dept. of Chemistry, University of Oregon, Eugene, OR 97403, fax: 541-346-5859*

Using vibrational spectroscopy to study adsorption at liquid surfaces is challenging, particularly if one wants to measure the surface properties with monolayer sensitivity. Nevertheless such measurements are important as liquid/air and liquid/liquid interfaces play a central role in a wide variety of physical, chemical and biological processes in our everyday lives. In this talk I will summarize some of our recent experiments that measure the vibrational spectroscopy of surface molecules at air/water and organic/water interfaces during monolayer formation. The spectroscopic technique employed in making these measurements is vibrational sum frequency spectroscopy (VSFS). The talk will summarize recent results that we have obtained in measuring the molecular structure of surfactants at liquid/air and liquid/liquid interfaces and the accompanying change in hydrogen bonding of water in the surface region. All of the studies described provide unique information about these interfaces, factors that control adsorption and monolayer formation and differences between the structure and adsorption at air/water and organic/water interfaces.

192.

USE OF MESOPOROUS SILICA IN CHIRAL HPLC. *Christopher C. Landry, Andrew G. Eklund, Sara T. Jull, and Karl W. Gallis. Department of Chemistry, University of Vermont, Cook Physical Sciences Building, Burlington, VT 05405, cclandry@zoo.uvm.edu*

Porous silica is commonly used as a matrix for chromatographic separations. The surface areas of commercially available chromatographic grade silicas are generally less than 500 m²/g. Mesoporous silica, which can have a surface area in excess of 1500 m²/g, is expected to provide superior separating ability. Mesoporous silica is prepared by a micelle-templated sol-gel process which produces pore diameters adjustable between 20 and 300 Å with narrow pore size distribution. The mesoporous surface can be modified by bonding various organic groups to the surface to affect separation of various species. We have performed achiral separations using a variety of mesoporous stationary phases, with excellent results in terms of resolution and efficiency. Commercially available chiral stationary phases (CSPs) often are expensive, and are not always effective in separating enantiomeric mixtures. In this investigation, a variety of CSPs using mesoporous silica were developed. Several β-cyclodextrin-bonded CSPs were shown to effectively separate enantiomeric mixtures of amines as well as other molecules.

193.

GOLD PARTICLES AS TEMPLATES FOR THE SYNTHESIS OF HOLLOW POLYMER CAPSULES: CONTROL OF CAPSULE DIMENSIONS AND GUEST ENCAPSULATION. *Stella M. Marinakos and Daniel L. Feldheim. Department of Chemistry, North Carolina State University, Campus Box 8204, Raleigh, NC 27695-8204, fax: 919-515-8909, emmarina@eos.ncsu.edu*

Colloidal gold is used as a template for synthesizing hollow poly(pyrrole) and poly(N-methylpyrrole) nanocapsules with excellent control over shell thickness and core diameter. Diffusion rates of the gold etch solution [0.1M KCN/0.001M K₃Fe(CN)₆] were found to depend on the oxidation state of the polymer. The gold particle is also shown to be useful in delivering molecules into the core of the capsule, allowing this procedure to be used as a method of encapsulation.

radable Analysis correlating morphology and deformation behavior in biodegradable lamella surface derived from oiled soapstock. PMSE 0138
 Biodegradable lamella surface derived from oiled soapstock. AGFD 0097
 Controlled insulin release from biodegradable phase transition polymer. DLY 0346
 Cyclization of biodegradable polymers and block-copolymer modification. CHED 0435
 Design and performance of poly(HPMA) hydrogels containing symmetric. POLY 0362
 Introduction of metal-binding units into biodegradable polymers utilizing. POLY 0333
 Natural fiber-reinforced biodegradable matrix composite: Effect of surface. PMSE 0033
 Symmetrical, biodegradable cross-linkers based on lactic or glycolic acid. ORGN 0394
 Tailored biodegradable properties of starch-based materials and their. BTEC 0029
 Toward the commercialization of biodegradable plastics in Japan: Materials. BTEC 0027
 Biodegradation induced PVT changes in oil-nmmed gas accumulation. GEOC 0050
 Biodegradation kinetics of BTEX in a compost biofilter. BIOT 0048
 Deep water exploration meets the largobiosphere: Biodegradation rates. GEOC 0009
 Drugs in municipal sewage effluent: Screening and biodegradation studies. ENVR 0044
 Effects of biodegradation on wax properties in the Gulf of Mexico. GEOC 0101
 Extraction study for enhanced biodegradation of petroleum hydrocarbon. ENVR 0150
 MTBE and benzene biodegradation by PM1 via two independent mechanisms. ENVR 0228
 Spatial disorder and degradation kinetics in intrinsic biodegradation systems. ENVR 0112
 Fluid communication inference among heavy, biodegraded oils using. GEOC 0074
 Biodesulfurization of gasoline: An assessment of technical and economic. I&EC 0269

tribution Synthesis and biodistribution studies of radioiodinated 1,1-dialkyl-4- MEDI 0205
 Bioeffect-related analysis. AGRO 0126
 Bioenergetics in cell-free protein synthesis systems. BIOT 0090
 Bioengineered polymers: Tailoring structure to control assembly and function. MACR 0030
 Bioengineered polysaccharides: Routes to control structure and function. BTEC 0024
 Dual species biofilm for bioremediation of the organophosphorus pesticide. BIOT 0312
 Reduction in pitting corrosion using regenerative biofilms on aluminum. BIOT 0315
 Biodegradation kinetics of BTEX in a compost biofilter. BIOT 0048
 Biofiltration for treatment of waste-gas mixtures containing chlorinated. I&EC 0270
 Importance of HPLC-MS in the analysis of bioflavonoids. AGFD 0180
 Kind of high-efficient biotoculant using for wastewater treatment. BIOT 0313
 Identification of β -damascenone progenitors and the possible biogenic. AGFD 0003
 Mechanism of TOPA quinone biogenesis. BIOL 0012
 Quinocofactor biogenesis in the copper amine oxidases: How does a. BIOL 0174
 Synthesis of the novel cytotoxic natural product WS9685B based on. ORGN 0040
 Advances in the analysis of biogenic polyamines using high-performance. ANYL 0017
 Analogs of a biogenic amine that exhibit cytotoxicity through induction. MEDI 0088
 Overview: The biogeochemical cycles of nitrogen and sulfur. INOR 0645
 Se biogeochemistry, ecotoxicology, and bioremediation. I&EC 0174

nic Biomobilization of mixed wastes. BIOT 0047

ormatics Beyond bioinformatics, R-D for drug discovery. COMP 0152
 Bioinformatics in the chemical-process industry. ANYL 0184
 Integrated view of bioinformatics for both genomics and proteomics. ANYL 0188
 Integrative bioinformatics: Bridging the chasm between genomics and. ANYL 0181
 Merging bioinformatics and chemoinformatics to map protein interactions. COMP 0150
 Signal transduction in insulin secretion: An opportunity for bioinformatics. ANYL 0187
 Trends, opportunities, and challenges in bioinformatics. ANYL 0180
 Single oxygen as a mechanistic tool in bioinorganic chemistry: The first. INOR 0075
 Investigation of phenolic biotransformation in opioids: Synthesis and. MEDI 0265
 Synthesis and stability studies of novel biotable products of 5-fluoro. MEDI 0056
 Studies of electron-transfer processes involving inorganic metal ions. INOR 0538

rganic Development of an integrated biochemistry and molecular biology methodology. CHED 0070
 Fluorocarbon-based organic materials as drivers for technological innovation. FLUO 0019
 General chemistry and cellular and molecular biology: An experiment in. CHED 0461
 Genomics, proteomics, and systems biology. BTEC 0009
 Integrative bioinformatics: Bridging the chasm between genomics and. ANYL 0181
 Merging chemistry and biology in the assembly of glycoproteins. CARB 0028
 Molecular imaging of the integrative biology of disease with PET. FLUO 0018
 Molecular modeling in biology and materials science: Prospects for the. COMP 0007
 New perspectives for NMR in structural biology using TROSY and CPMAS. PHYS 0011
 Using real-world questions in an integrated chemistry, biology, and. CHED 0202
 and Bioburial: The shear of adsorbed polyelectrolytes and of polymer. PMSE 0062
 Desomosterol: A biomarker for the potential wildlife contraceptive. AGRO 0092
 Biomarkers for tobacco-smoke exposure. TOXI 0016
 Comparison between geochemical parameters derived from biomarker. GEOC 0003
 Enantiomer separation of branched aliphatic alkane biomarkers. GEOC 0041
 Immunoassays as biomarkers of human exposure to toxins. AGRO 0107
 Monoterpenes in ponderosa pine as biomarkers of genetic diversity. ANYL 0141
 Quantitative analysis of oil biomarkers: Potential indicator of dynamic. GEOC 0063
 Release of functionalized biomarkers from oil asphaltenes via hydrophobic. GEOC 0036
 Application of room-temperature ionic liquids to the chemical process. I&EC 0002
 Biomass and renewable fuels. FUEL 0051
 Demonstration of ethanol production from cellulosic biomass. BTEC 0047
 Elucidating atmospheric SVOCs in agricultural biomass combustion. ENVR 0215
 Evaluation of an optical technique for monitoring biomass in plant cell. BIOT 0295
 Identification of maize cell-wall mutations using near-IR spectroscopy. BTEC 0052
 Numerical modeling of NO reduction using biomass pyrolysis-oil-based. FUEL 0058
 Overall approach to biomass-to-ethanol and other chemicals. BTEC 0044
 Renewable energy and energy efficiency: Using biotechnology and. BTEC 0019
 Strategies for successful metabolic engineering of *Saccharomyces cerevisiae*. BIOT 0119
 Thermoplasticization and liquefaction of biomass and their application. CELL 0040
 Tropospheric ozone formation from biomass burning and urban release. PHYS 0099
 Use of process analysis to evaluate economics, research priorities, and. BTEC 0045
 Structural design of bacterial cellulose as biomaterial in microsurgery. CELL 0012
 Biosynthesis of novel polysaccharide copolymers: New families of poly. CELL 0010
 Dye-modified cellulose: Biomaterials for optoelectronic applications. CELL 0070
 In situ forming polymeric biomaterials. MACR 0038
 Nanoporous thin films for biomaterials applications. COLL 0211
 New methods for preparation and analysis of cellulose and related poly. CELL 0032
 Poly γ -D-glutamic acid as a template for functionalized water-soluble. BIOL 0133
 Temperature-sensitive biomaterials for delivery of bone morphogenetic. BIOT 0354
 Use of combinatorial approaches in the design of novel biomaterials. MACR 0037
 Hydrogel polymers from alkylthio acrylates for biomedical applications. POLY 0529
 Preclinical methods for studying smoking behavior and its biomedical. TOXI 0011

Biomimetic approach to lignin degradation: Metalloporphyrins catalyze. CELL 0118
 Biomimetic CO₂ uptake reactions: Applications for the biotin-dependent. INOR 0756
 Direct electrochemistry of biological redox carriers in biomimetic. INOR 0615
 Electrochemistry and conducting polymers: Soft, wet, multifunctional. COLL 0372
 Formation of novel lead sulfide phases by a biomimetic synthetic route. INOR 0260
 Lessons from nature: Novel design strategies for biomimetic silica. INOR 0436
 Mechanistic studies of substrate activation by biomimetic nonheme diiron. INOR 0553
 New paradigm for cofactor regeneration, enzyme recognition of biomimetic. INOR 0660
 Simulation of biomimetic recognition between polymers and surfaces. PHYS 0087
 Synthesis of biomimetic marine natural products via enzymatic and. BIOT 0009
 Rational design of biomimetics with QM/MM Car-Parrinello simulation. PHYS 0334
 Biomolecular films with electrochemical and enzyme activity construct. COLL 0461
 Derivatized poly(L-lysine)-graft-poly(ethylene glycol) monolayers as. COLL 0396
 Metal nanoparticles chemically assembled on biomolecular scaffolds: INOR 0259
 Microfluidic patterning of SiO₂ surfaces with derivatized poly(L-lysine). COLL 0154
 Comparing the performance of prepacked columns and self-packed. BIOT 0199
 Copper-catalyzed N-arylations of small biomolecules with aryllead(IV). ORGN 0028
 Development of new therapeutics from microbial biosurfactants and. CARB 0080
 Low-density-array optical chips for multiplex detection of biomolecular. I&EC 0236
 Modification of electrodes with self-assembled monolayers and by so. ANYL 0139
 Neurite outgrowth on microscale patterns and gradients of biomolecular. BIOT 0014
 Reactivity studies of antitumor active dirhodium carboxylate complexes. INOR 0081
 Rupturing biomolecules with the AFM: Single-molecule bond rupture. COLL 0313
 Second harmonic generation of chiral biomolecules in biological membranes. PHYS 0191
 Self-assembled bisbenzamide mono- and bilayers: Reversible selection. COLL 0460
 WebCT-based biomolecules tutorial module for general chemistry. CHED 0956
 X-ray absorption spectroscopy (XAS) as a tool to study sulfur-containing. INOR 0520
 Use of prototype runs to address integration of different steps in biop. BIOT 0122

biomimetics Biomolecular Biopharmaceutical Biopharmaceuticals Biophysics Biopolymer Bioprocess Bioprocessing Bioprospecting Bioreactor Bioreactors Biorecognition Bioremediation Biorenewable biosensors Biosensing biosensor biosensors Bioprocession Bioprospecting Bioreactor Bioreactors Biorecognition Bioremediation Biorenewable biosensors Biosensing biosensor biosensors Bioprocession Bioprospecting Bioreactor Bioreactors Biorecognition Bioremediation Biorenewable biosensors Biosensing biosensor biosensors Bioprocession Bioprospecting Bioreactor Bioreactors Biorecognition Bioremediation Biorenewable biosensors Biosensing biosensor biosensors

Biopharmaceuticals in the 21st century: Changes and challenges. BIOT 0057

Silicon proteomics: From protein biophysics to protein biochips. I&EC 0197
 Synthesis and biophysics of triple helical collagen mimetics. POLY 0574
 Natural fiber-reinforced biodegradable matrix composite: Effect of surface. PMSE 0033
 Exploring biopolymer structure and function through aqueous dynamics. CELL 0065
 Is HCN polymer the primordial biopolymer?. GEOC 0056
 Polymer Processing in Microgravity: Biopolymer production under simulated. POLY 0619
 Polymeric Bioconjugates: Genetically engineered biopolymer conjugates. POLY 0580
 Suberin: A nonlipid plant cell-wall phenolic biopolymer. CELL 0117
 Biopolymers. MACR 0010
 Cellulose ester biopolymers in the 21st century. MACR 0028
 Enzymatic method to create functionalized biopolymers. BIOT 0293
 Thermoreversible and irreversible physical gels from biopolymers. POLY 3004
 All-in-one bioprocess monitoring with a mid-IR spectroscopic sensor. BIOT 0363
 Bioprocess integration in the production of a novel enzyme system to. BIOT 0125
 Economic aspects for the bioprocess equipment design/selection. BIOT 0371
 Increasing bioprocess optimization efficiency by identification of critical. BIOT 0328
 Integration of development and engineering concepts for a successful. BIOT 0367
 Green fluorescent protein as a paradigm for integrated bioprocessing. BIOT 0128
 Hydrophobic displacement chromatography (HDC): Applications for biop. BIOT 0154
 Bioprospecting for novel aromatic oxygenases. BIOT 0001
 Artificial liver in a pulsating pinch-flow hollow-fiber bioreactor. BIOT 0265
 Bioreactor characterization and scale up in cell culture fermentation. BIOT 0357
 Effect of culture in a rotating wall bioreactor on physiology of neuronal. BIOT 0266
 Engineering *Escherichia coli* cell surface for detoxification of organophosphorus. AGRO 0023
 Increased foreign protein production and recovery from plant cells cultured. BIOT 0023
 Investigation of the gas balance in microbial fermentations performed. POLY 0437
 Optimization using a scaled-down hollow-fiber bioreactor. BIOT 0358
 Potential use for polymers in bioreactor systems. I&EC 0136
Escherichia coli bioreactors as multicellular organisms via quorum sensing. BTEC 0036
 Fate of ampicillin in the growth of recombinant *E. coli* in bioreactors. BIOT 0238
 Monitoring and modeling of bioreactors for mammalian cell culture use. BIOT 0364
 Scale up and scale down between bench, pilot, and production bioreactors. BIOT 0366
 Serum-free media development for MAb production in high cell density. BIOT 0172
 Porphyrin self-assembly on gold for molecular design of biorecognition. COLL 0399
 Bioremediation of chelated Cu(II) ion by bacteria: A comparative study. ENVR 0171
 Dual species biofilm for bioremediation of the organophosphorus pesticide. BIOT 0312
 Enhanced bioremediation pilot study for chlorinated solvents in karst. I&EC 0219
 In situ bioremediation of MTBE: Lessons from laboratory experiments. ENVR 0121
 Lab-scale model for in situ bioremediation of a carbon tetrachloride-. I&EC 0218
 Se biogeochemistry, ecotoxicology, and bioremediation. I&EC 0174
 Solving the Panoche Fan selenium pollution using an unconventional. I&EC 0169
 Use of ORC in the bioremediation of MTBE. ENVR 0233
 New single-site catalysts for the synthesis of polyesters and polycarbonates. MACR 0022
 Combining living cells with electronics for versatile biosensors. TOXI 0030
 Biosensing based on b-cells with transfected aequorin. TOXI 0029
 3-D cultures of primary neural cells for tissue-based biosensor. TOXI 0031
 Detecting microorganisms in water using the AMBRI ion channel-swing. ANYL 0204
 Detections of DNA damage using a fiber-optic biosensor. ANYL 0205
 DNA biosensor: Immunosensor applications for anti-DNA antibodies. I&EC 0215
 Human toxicity to aflatoxins: Biological potency and biosensor detection. TOXI 0026
 Biosensor a viable method for food allergen detection?. AGRO 0116
 Rapid detection of recombinant proteins in cell extracts using a gene. BIOT 0272
 Tyrosinase-based carbon-paste electrode biosensor for detection of. ANYL 0111
 Amperometric enzyme biosensors for field monitoring of organophosphorus. ANYL 0239
 Detection of toxic events in hepatocyte biosensors. TOXI 0033
 Evaluation of small-scale quartz-crystal microbalance and surface-potential. ANYL 0203
 Miniaturized biosensors by in situ assembly of colloidal particles onto. COLL 0393
 Monte Carlo simulations of photon propagation in poly(ethylene glycol). ANYL 0142
 Redox-active photophosphazenes and their application as electron-transport. POLY 0273
 Microfiltration-based integrated bioseparation processes: Case study. BIOT 0123
 Bioseparations using complex systems and micromanufacturing techniques. I&EC 0029
 Controlled surface structure to prepare ion-exchange phases for biosensing. BIOT 0183
 Charge ladders of proteins and capillary electrophoresis measure. BIOT 0339
 Anomalous fractionation of oxygen isotopes in stratospheric carbon dioxide. PHYS 0205
 Development of new therapeutics from microbial biosurfactants and. CARB 0080
 Assembling and exploiting nature's chemical arsenal: Calicheamicin biosynthesis. ORGN 0690
 Biochemistry of natural rubber biosynthesis. CELL 0135