

# The Laboratory Robotics Interest Group Mid Atlantic Chapter

## May 2010 Meeting

### The Sixteenth Annual Technology Posters

#### VENDOR MEMBERS

Unique cellular signatures for predictive compound profiling using high-content analysis of signaling networks

Thomas Koblizek (1), Ann Siehoff (1), Anthony Pitt (1), Leon De Bruin (1), Alex Batchelor (1), Jane Lamerdin (2), John Westwick (2), Nicole Faust (1).

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(2) Odyssey Thera, Inc., 4550 Norris Canyon Road, San Ramon, CA 94583, USA.

Modern drug discovery workflows seek to address the specificity of drug/target interactions, but often fail to reflect the inherent complexity of the protein complexes and biochemical networks within the live cell context missing key “off target” effects. A major challenge for drug discovery remains the need for assays that capture diverse targets and pathways in their native state delivering a picture of the global cellular response to a drug candidate. We have created a cell based systems biology platform that moves beyond classical off-target profiling methods and enables us to learn much more about lead compounds, their mode of action and possible future dangers. The platform comprises a panel of cell based protein-protein interaction measurements facilitating analysis of known signaling pathways in a highly contextual fashion.

Using this platform we assessed the system-wide activity of hundreds of diverse known drugs, failed drugs, toxicants, and genetic reagents. We observed that all drugs and toxicants, including closely-related chemical structures, generate a unique “signature” across the panel. Compounds with similar mechanisms of cellular toxicity generated reproducible signatures, enabling the development of algorithms which predict selectivity, safety, and efficacy of novel therapeutic candidates.

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LRIG Mid-Atlantic 2010 Abstract

Is Your Automated Liquid Handler Working For Your Assays – Uncovering Errors, Understanding Device Behavior, and Optimizing Methods

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Keith J. Albert

Artel, Inc., 25 Bradley Drive, Westbrook, Maine 04092

The focus of this presentation is to highlight the need of ensuring quality in important assays performed with automated liquid handlers. Nearly all assays performed within a laboratory are volume-dependent. In turn, all concentrations of biological and chemical components in these assays, as well as the associated dilution protocols, are volume-dependent. Because analyte concentration is volume-dependent, an assay's results might be falsely interpreted if liquid handler variability and inaccuracies are unknown or if the system(s) go unchecked for a long period. Measuring and knowing the exact volumes transferred, for specific and/or routine methods, will inherently lead to confidence in the experiment, i.e., the results can be trusted.

This presentation focuses on the importance of understanding liquid handler behavior for many types of assays. To understand and assess liquid handler performance in each case, a standardized volume verification method was employed (MVS® Multichannel Verification System). For instance, it will be presented how the liquid handling steps were measured, understood, and/or optimized: (1) on-board mixing efficiency; (2) finding a bad "tip-in-the-box" in a newly opened tip box; (3) highlighting the differences between accuracy and precision; (4) comparing individual volume transfers over multi-sequential dispenses; (6) optimizing an automated method for a specific target volume; and (7) directly comparing performance between liquid handlers from multiple locations.

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Evaluating Five Microplate Mixing Techniques – Diffusion, Centrifugation, Shaking, Pipetting and Ultrasonic Mixing

Jean Shieh, Bruce Jamieson and Vibhu Vivek; Microsonic Systems, Inc.

Drug discovery miniaturization efforts have been successful at dramatically increasing the density of microplate assays, substantially reducing assay volumes but inadvertently adding physical difficulties regarding adequate mixing of the assay components. As microplate well volumes decrease, variables such as surface tension and the aspect ratio of taller, thinner wells have raised concerns about the effectiveness of traditional mixing techniques. To address this, Microsonic Systems has developed the HENDRIX SM100 specifically for mixing, solubilization and suspending liquids in 96, 384, 1536 well formats and beyond. Microsonics has recently developed a methodology to evaluate the thoroughness of microplate assay mixing and used it to characterize the effectiveness of mixing in 384 well microplates with five common mixing

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techniques: diffusion, centrifugation, shaking, pipetting as well as ultrasonic mixing with our own HENDRIX SM100. The method is simple, yet precise and accurate, and it uses standard drug discovery tools such as single- and multi-channel pipettes, an automated liquid handler and a UV/Vis microplate spectrophotometer. This poster describes the method and results of these five mixing alternatives.

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#### Improve the Integrity of Your Fragment Library for Fragment-Based Drug Discovery

Jean Shieh, Vibhu Vivek, Bruce Jamieson and Justin Bramwell, Microsonic Systems Inc.

Fragment-based drug discovery (FBDD) is gaining recognition due to its many advantages over high-throughput screening such as better hit-to-lead rate and the broad chemical space for possible compound scaffolds. Due to the low affinity of fragments to the biological target, fragment libraries may contain weak hits and therefore scientists screen fragment libraries at concentration as high as 200 mM. Even though many fragments have high solubilities in DMSO, environmental shocks introduced by DMSO hydration or repeat freeze/thaw cycles can cause compounds to crash out of solution, and consequently affect the accuracy of the FBDD screening results. To address this issue, Microsonic Systems has developed HENDRIX SM100 Ultrasonic Fluid Processor specifically for solubilization, thawing, and mixing; compound precipitates can be solubilized in just a few minutes with the HENDRIX SM100. In this poster, we will present the outcome of a solubilization study for fragment libraries. We will also look at how ultrasonic fluid processing improves the assay results.

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#### Rapid Exploration of Chemical and Biological Space: New Approaches, Informatics, Robotics and Libraries

**Melvin Reichman, PhD., Scott Donover, Amanda R. Schabdach, et al.**

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Lankenau Institute for Medical Research Chemical Genomics Center (Wynnewood, PA)

#### ABSTRACT

The confirmed 'hit rate' for typical HTS assays is less than 0.5%; therefore, 99.5% of the costs of HTS are for generating null data. We are collaborating to refine an approach to primary HTS that is 500% more efficient than present practice referred to as orthogonal pooled screening (OPS). The OPS method is an intelligent pooling approach that combines ten (10) compounds per well across two independent orthogonal matrices, with each compound represented twice in two separately arrayed pools, mixed with a different set of nine other compounds at each location. This duplication improves the validity of statistical interpretation of the HTS data and greatly simplifies verification by de-convolution of true actives. *The Lankenau Chemical Genomics Center (LCGC)* has developed an innovative infrastructure to produce and distribute novel compression libraries of hundreds of thousands of small molecules for parallel HTS campaigns, de-convolute the screening hits, and then rapidly resupply individual active compounds. **LCGC offers free sets of 8,000 drug-filtered diverse compounds, pre-formatted for new collaborators to test the OPS approach for novel assays in their lab. Please contact [reichmann@mlhs.org](mailto:reichmann@mlhs.org) for details.**

NOTE, THERE ARE TWO ADDITIONAL VENDOR POSTERS FOR WHICH WE DO NOT HAVE TITLES OR ABSTRACTS. ONE WILL BE PRESENTED BY Amy Mitchell of SRU Biosystems, and the other will be a second poster presented by Thomas I. Koblizek of Lonza Cologne AG.

#### STUDENTS:

Kelly Carman & Kristina Petrie, Morristown High School

Using aromatherapy to decrease stress levels in medical practitioners by utilizing salutogenic methods

Julia Pikus, Morristown High School

Using classical music as an environmental enrichment tool for kenneled canines

Laura Rolon, Morristown High School

A measure of Homo sapien molar erosion rates caused by energy drinks

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Tim Carroll, Morristown High School

Testing the effectiveness of hypnopedic teachings on adolescents

Catherine Wong, Morristown High School

Novel Foot-Pedal Powered Device for Generation of Light in Impoverished Areas

Daniel Knapp, Morristown High School

"Eco-Friendly" hazards: Examining bacteria propagation in refillable, aluminum water bottles

Marvin Castellon, Union City High School

Use of nitrocellulose as a solid support in immunoaffinity chromatography

Paola Severino, Union City High School

Lanthanoid complexes; constructing a magnetic resonance imaging contrast agent

Emma Russo, Union City High School

New chemistry with isosorbide

Kevin Erazo, Union City High School

Hybridization of oligonucleotides leading to formation of a cube like structure

Shobika Sivaram, Union City High School

Synthesis of benzylidene acetals of d-glucal

Luis Mendez, Union City High School

Electrophoresis deposition of carbon nanotubes

Walter Echevarria, Union City High School

Novel antibacterial activity from the leaves of asclepias incarnata

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Danny Palacios, Union City High School

Light intensity light power measurements of homogeneous dielectric barrier discharge

Hager Mohamed, Union City High School

The effect of oreganum vulgare on h.pylari

Dinusha Kalupehana, Union City High School

Cloning dna il-10

Adam Schwing and Ronak Patel, JKF Memorial High School

Optimizing Growth Media and Bioreactor Design for Hydrogen Production in *C. reinhardtii*

#### **JOHN MORIN MEMORIAL SCHOLARSHIP RECIPIENTS**

Saagar Deshpande, Livingston High School, Plans to study Biology and Computer Science at Columbia University.

Kevin Hardy, Home Schooled, Plans to study Chemical Engineering, Accepted at Penn State, University of Virginia, Northwestern, and Cornell but has not yet made a decision.

Kathryn Todd, Rancocas Valley Regional High School, Plans to study Aeronautical Engineering at Embry – Riddle Aeronautical School.

Lauren Nowicki, Hopewell Valley Central High School, Plans to study Physics and Education at Gettysburg College