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REGIONAL ACADEMIC DRUG DISCOVERY SYMPOSIUM

Tomorrow's Drugs Today

November 8, 2017
NJCSTM Building, Kean University

1075 Morris Avenue, Union NJ 07083

08:45 AM Welcome and Opening Remarks

Keith Bostian, Ph.D. CEO, Institute of Life Science Entrepreneurship & Dean, NJCSTM Program and Office of Tech Transfer, Kean University

09:00 AM Session 1 : Different Collaboration Models

09:00 AM Tri-I TDI/Bridge Medicines: a novel academic drug discovery and development model

Bruce R. Conway, Ph.D. Director, Rockefeller University & The Tri-Institutional Therapeutic Discovery Institute

Bruce Conway is the Director of the Robertson Therapeutic Development Fund at Rockefeller University. He is also a member of the SAB for the Tri-Institutional Therapeutic Discovery Institute, a collaboration among MSKCC, The Rockefeller University, Weill Cornell Medicine and Takeda, to advance the groundbreaking discoveries of the academic institutions.

Bruce earned his PhD. in Pharmacology at the Medical College of Virginia and completed his postdoctoral fellowship at the University of Massachusetts Medical Center. He then joined Johnson & Johnson Pharmaceutical Research and Development where he championed the progression of three compounds into the clinic, one of which resulted in the FDA approval of a novel, first-in-class treatment for Type 2 diabetes Invokana®. In 2006, he moved to the Institutes for Pharmaceutical Discovery as the Senior Director of Biology where he oversaw the day-to-day operations of the Biology, Pharmacology and DMPK teams.

In 2013, Bruce transitioned to academia and served as the "Executive-in-Residence" at Columbia University. The following year, he joined the Rockefeller University where he serves in his current position. He serves on the Faculty within the Clinical Center for Translational Science and as an advisor to Pfizer's Center for Therapeutic Innovation, Columbia Technology Ventures, the Coulter Translational Research Boot Camp and 1st Pitch Life Sciences NYC.

09:25 AM Bootstrapping Translational Research in Academia - Rutgers University Experience

David Kimball, Ph.D. Assoc. Vice President, Translational Sciences and Research Commercialization, Rutgers University

David Kimball is Associate Vice President of Rutgers Translational Sciences and Research Commercialization, in the Office of Research and Economic Development. He is also a Research Professor in the Ernest Mario School of Pharmacy. David obtained his PhD in Organic Chemistry/Chemical Biology from the State University of New York at Stony Brook, and spent the first 19 years of his career at Bristol-Myers Squibb Pharmaceutical Research Institute, leading drug discovery and development efforts in cardiovascular medicine and oncology.

In 2001 he moved to Lexicon Pharmaceuticals in Princeton, NJ as Vice President of Chemistry and directed discovery and development chemistry efforts for Lexicon's entire small molecule clinical pipeline. Prior to joining Rutgers University, David also served as Senior Vice President of Nonclinical Research at Pharmacopeia, Inc., and Chief Scientific Officer of Hydra Biosciences, in Cambridge, MA

09:50 AM **The Moulder Center for Drug Discovery Research - Integrating the Best of Academia & Industry**

Wayne Childers, Ph.D. Associate Professor, Temple University School of Pharmacy and The Moulder Center for Drug Discovery Research

Wayne Childers is Associate Professor of Medicinal Chemistry at Temple University School of Pharmacy, Philadelphia, PA and Associate Director of the Moulder Center for Drug Discovery Research. Wayne received his BA from Vanderbilt University in chemistry in 1979 and a PhD in organic chemistry from the University of Georgia in 1984. He served as an Assistant Adjunct Professor at Bucknell University before accepting a position as a postdoctoral fellow at the Johns Hopkins University School of Medicine.

Wayne then joined Wyeth Research, Inc.in 1987, working for over 23 years as a medicinal chemist in numerous therapeutic areas, including psychiatric diseases, stroke, epilepsy, Alzheimer's disease, and the treatment of chronic pain. Teams under his leadership delivered 4 compounds to clinical trials. Wayne then accepted his present position at Temple University in 2010. Wayne is an author on over 50 peer reviewed papers, reviews and book chapters and is an inventor on 40 US patents.

10:15 AM **Translating Academic Innovation into Commercial Opportunity through LIBH REACH Program**

Li Liu, Ph.D. Assistant Director, Business Development, Center for Biotechnology, Stony Brook University

Li provides technology commercialization and business development services to facilitate new venture creation and support emerging company growth. Currently, Li is working with a dozen New York state based startup companies across the Life Sciences Industry. Li is also a core member of Long Island Biosciences Hub (LIBH), which was formed after the NIH Research Evaluation and Commercialization Hub (REACH) award (three awardees across the country) was received.

Li manages the technology development fund to invest in promising therapeutics, diagnostics, medical devices, research tools and healthcare IT projects across Stony Brook University, Cold Spring Harbor Laboratory and Brookhaven National Laboratory and help the innovations into the commercial sector via startup companies, licensing opportunities, and/or strategic partnerships. Li received his B.S. in Chemistry from Fudan University in China and Ph.D. in Chemistry from Stony Brook University.

He has also passed CFA level III exam (CFA expected 2018) and is alumni of Fundamentals of the Biosciences Industry Program. Prior to joining the Center he worked at Ascent Biomedical Ventures and Forest Laboratories conducting due diligence on investment/M&A opportunities.

10:40 AM **Break**

11:15 AM Session 2 : Funding Translational Research

Ordinarily, academic funding is difficult to obtain for other than for basic research. To fund advanced efforts and move down the path to IND, support from groups such as Venture Capital (VC), angel investors, foundations or pharma/biotech needs to be obtained. Understanding what each of these groups are looking for and when might be a good time to approach them will be helpful. This session will be conducted in panel format to maximize utility to the audience using Q&As. The start of the session will be a short introduction from each the 4 panelists representing VC, angel, pharma and foundation.

Session chair – Vincent Smeraglia, J.D., Executive Director, Office of Research Commercialization, Rutgers University

Vincent A. Smeraglia, Esq. is the Executive Director, Strategic Alliances, developing Rutgers collaborative relationships with universities, foundations, and corporate partners. Previously, Mr. Smeraglia was the Executive Director of the Rutgers office of Technology Commercialization overseeing patenting and licensing of Rutgers inventions.
Mr. Smeraglia was also the Executive Director of the UMDNJ Office of Technology Transfer & Business Development. He has also conducted biomedical research at Cytogen Corporation, developing antibody conjugates for diagnostic and therapeutic clinical uses. Mr. Smeraglia has a B.S. in Biochemistry from Rutgers and a Masters of Intellectual Property and J.D. from the University of New Hampshire Law School.

Peter Alff, Ph.D., Executive in Residence, Kairos Ventures

In his role as Executive in Residence at Kairos Ventures, Peter works directly with founding scientists and their teams to develop and execute both scientific de-risking and commercialization strategies for Kairos portfolio companies. Peter provides management and business development guidance, enabling these companies to readily define and negotiate potential risks while maximizing progress towards key scientific and commercial milestones. Peter brings over a decade of experience in translational science, business development, and startup operations with an emphasis on early-stage life science and biotechnology companies. Peter has been a founder and Director of Strategic Initiatives for a biotechnology and protein-engineering company, leading programs that raised millions of dollars.
As a former Business Development Manager for NYU's Office of Therapeutics Alliances, Peter has facilitated company formation based on university technology across multiple therapeutic areas, including oncology, auto-inflammation, neuroscience and infectious disease, and brings significant expertise in the nuanced process of translating university research and intellectual property into commercially viable ventures. Peter completed his postdoctoral training at The Rockefeller University, received his PhD in Molecular and Cellular Biology from Stony Brook University, and completed his undergraduate studies at Muhlenberg College where he received a B.S. degree in Biology.

Stephen Goodman, JD, Co-Founder, Mid-Atlantic Bio Angels

Stephen M. Goodman is a co-founder of Mid Atlantic Bio Angels (www.bioangels.net), an angel investor group, and 1st Pitch Life Science (www.1stpitchlifescience.com), a public forum for pitches from pre-investment stage companies, in each case for companies in the life sciences. He has mentored numerous life science and technology start-ups through The Eugene Lang Entrepreneurship Center at Columbia Business School, the Columbia-Coulter Translational Research Partnership, the Bench-to-Bedside Initiative of Weill-Cornell Medical Center, Memorial Sloan Kettering Cancer Center and Rockefeller University and the E-Lab for Life Science Entrepreneurs sponsored by the New York City Economic Development Corporation.

Steve is also a partner and co-head of the Life Sciences Group at Pryor Cashman a law firm in New York City. His clients include drug development and diagnostic companies, medical device companies, clinical trial management companies and companies in other technology businesses. He is a member, and has served as the chair, of the Biotechnology Law Committee of the American Bar Association's Science and Technology Law Section, and sits on the editorial board of The SciTech Lawyer, a popular publication of that section.

Carolyn Buser-Doepner, Ph.D., VP and Global Head of Discovery Partnerships with Academia, Glaxo Smith Kline R&D

Carolyn A. Buser is Vice President of Discovery Partnerships with Academia at GlaxoSmithKline. She received her B.A./B.A. in chemistry and German from Bryn Mawr College, spent one year as a Fulbright Scholar at the Technical University of Braunschweig in Germany, and obtained her Ph.D. in Biophysical Chemistry at Yale University in 1992. She was a Damon Runyon – Walter Winchell postdoctoral fellow at the State University of NY at Stony Brook and subsequently served as Research Assistant Professor. In 1996, Carolyn joined the Oncology group at Merck Research Labs, holding positions as pre-clinical team leader for several drug discovery programs, director of Oncology Health Care Solutions, and finally senior director of External Scientific Affairs in Oncology.

In March 2011, Carolyn joined GlaxoSmithKline (GSK), where she now leads a team of drug development scientists who identify and progress novel targets in partnership with biology and disease experts in academia. Within GSK, she co-chairs the GSK Fellows Program and is a member of the Technology and Discovery Investment Boards. Carolyn is a member of AACR and AAAS and is bilingual in German.

James Golubieski, President, NJ Health Foundation/Foundation Venture Capital Group

James M. Golubieski is President of New Jersey Health Foundation and its affiliate, Foundation Venture Capital Group, LLC, a company that provides pre-seed funding to new health-related startup companies founded by New Jersey researchers to help them advance toward commercialization. Jim works closely with the companies in which Foundation Venture has invested, sits on their Boards and provides guidance in helping them to develop their business models.

Previously he had been CFO of Array Medical, Inc., a medical device start-up company established in 1995 that developed a groundbreaking blood test to test platelet function. The company was sold in 1999. Jim was also the chief operating officer and senior executive vice president of Glendale National Bank and a member of its board of directors, president of Glendale Investment Corp. and Glendale Mortgage Services, Inc. and chief financial officer of Glendale Bancorp, which was acquired by Mellon Financial., For 10 years prior he had been with KPMG.

12:15 PM **Lunch and Poster Session: Topics in Academic Drug Discovery**

02:00 PM **Session 3 : Case Studies**

02:00 PM **Trigriluzole: An SBIR-Derived Clinical Compound for the Treatment of Neurological Diseases and Melanoma**

Allen Reitz, Ph.D. CEO, Fox Chase Chemical Diversity Center

Allen Reitz is CEO and founder of the Fox Chase Chemical Diversity Center, Inc. (www.fc-cdci.com) with laboratories in Doylestown and King of Prussia, PA. FCCDC is an early-stage translational research organization with a core competency in target validation, hit to lead and lead optimization medicinal chemistry. He has had >35 years of experience in the pharmaceutical industry, including nearly 26 years with Johnson & Johnson. He has developed 8 compounds that have entered human clinical trials. He has >140 scientific publications and 61 issued U.S. patents, and is the Editor-in-Chief of the journal Current Topics in Medicinal Chemistry.

He has extensive experience in project and portfolio management, target validation, hit triage, hit to lead and lead optimization medicinal chemistry, eADME profiling, and preclinical candidate selection. He is also Adjunct Professor at Drexel University College of Medicine, holds an Executive Masters in Technology Management from the University of Pennsylvania (Wharton, Penn Engineering), and is a Moore Fellow in the Management of Technology (U. Penn.). Dr. Reitz is also a founder and CEO of ALS Biopharma, LLC, focusing on the neurological condition of amyotrophic lateral sclerosis.

02:30 PM **CX3CR1 Chemokine Antagonists Halt Metastatic Spreading in Animal Models of Metastasis**

Joseph Salvino, Ph.D. Professor, Medicinal Chemistry, The Wistar Institute

Joe Salvino is currently at The Wistar Institute, Philadelphia, PA. He received his Ph. D. from Brown University with Prof. Paul G.Williard and Postdoc'ed with Professors KC Nicolaou and Ralph F. Hirschmann at the University of Pennsylvania. His expertise is in medicinal chemistry, with over twenty years experience. He is currently focusing on early stage in vivo pharmacological target validation, hit to lead, and lead optimization to provide value to Academic Drug Discovery programs.
Joe has been involved in three start-up companies: Alliance Discovery, Inc, Kerberos Biopharmaceuticals, Inc, and Context Therapeutics, Inc. the latter two spun out of Drexel University College of Medicine. Joe had a Project leader role in several pharmaceutical companies, successfully optimizing and providing development candidates, several of these candidates have successfully completed human phase I and phase II clinical trials, including Entereg®, ADL-101, and Radezolid®. Expertise: High Throughput Chemistry/ Hit to Lead/ Lead Optimization Medicinal Chemistry / Rational Drug Design.

03:00 PM **ILSE-CTM-ATCC Partnership: The Evolution of an Idea into Products used in Drug Discovery**

Tasha M. Santiago-Rodriguez, Ph.D. Scientist and Team Leader, ATCC-Center for Translational Microbiology

Dr. Tasha Santiago-Rodriguez is a scientist and team leader at the ATCC-Center for Translational Microbiology (ATCC-CTM), where she joined in 2016. Her current role involves the development and implementation of spike-in standards in microbiome research. Dr. Santiago-Rodriguez received a Ph.D. from the University of Puerto Rico in Public Health Water Microbiology. She moved to San Diego for a postdoctoral appointment at the University of California to work on diverse areas of human microbiome research.

There, she worked in the characterization of the meta-transcriptome profiles of Methicillin-Resistant Staphylococcus aureus (MRSA) bacteriophages in the human bloodstream, microbiome and virome profiles in association with urinary tract infections, and short and long-term effects of antibiotics to the human gut and oral virome. Dr. Santiago-Rodriguez was also a recipient of a prestigious postdoctoral fellowship from the Howard Hughes Medical Institute to work in the characterization of ancient human gut and oral microbiomes, viromes and resistomes.

03:30 PM **Networking and Refreshments**

05:00 PM **Adjourn**

Poster Abstracts

1. Zinc metallochaperone complexes that restore wildtype structure and function to mutant p53

Xin Yu[2], Bing Na[2], Yue Liu[2], Anthony Bencivenga[1], John A. Gilleran[1], David J. Augeri[1], Meagan Hackey[1], S. David Kimball[1], Adam Blanden[3], Stewart Loh[3], Darren R. Carpizo[2]

(1) Molecular Design and Synthesis, Rutgers Translational Sciences and Dept. of Medicinal Chemistry, EMSOP, Rutgers, Piscataway, NJ
(2) Dept. of Surgical Oncology, Rutgers Cancer Institute of New Jersey, New Brunswick, NJ
(3) Dept. of Biochemistry and Molecular Biology, SUNY Upstate Medical University, Syracuse, NY

The Molecular Design and Synthesis group, of Rutgers Translational Sciences, performs synthesis of probe molecules in collaboration with Rutgers/CINJ PIs to study novel biology. We have 7 established programs and 4 early phase programs. Preliminary results were obtained for the p53 reactivator program ZMC1 was studied as a zinc-binding monomer. Also, stable neutral zinc complexes were studied. X-ray structures served to strengthen experimental stoichiometry such that two ZMC1 ligands in complex with a Zn2+ ion form the stable, neutral complex, Zn-1. This neutral complex enters the cell to deliver Zn2+ to the mutant p53 protein and allow it to re-fold to return it to its natural conformation and function. The SAR of ZMC1, the structures of the 1:2 complex, cell-based experiments plus in vivo efficacy studies comparing the monomer ZMC1 to the complex Zn-1 served to strengthen the NIH R01 grant proposal that was funded, **NIH-NCI R01CA200800**, 2.09M (2015-20). These results are presented herein.

2. Molecular Design and Synthesis Group, Rutgers Translational Sciences

David J. Augeri[1], John A. Gilleran[1], Rachael Bigos[1], Cindy Kui[1], Raheel Fondekar[1], S. David Kimball[1], Monica Bartucci[1], Nitu Bansal[2], Vince Smeraglia[1], Hatem E. Sabaawy[2], Purnima Bhanot[3]

(1) Molecular Design and Synthesis, Rutgers Translational Sciences and Department of Medicinal Chemistry, Ernest Mario School of Pharmacy, Rutgers, Piscataway, NJ
(2) Rutgers Cancer Institute of New Jersey, New Brunswick, NJ
(3) Dept. of Medicine, Rutgers-Newark, NJ

The Molecular Design and Synthesis group, of Rutgers Translational Sciences, performs synthesis of probe molecules in collaboration with Rutgers Principal Investigators to study novel biology. This effort helps to obtain preliminary results and proof of principle in novel programs to strengthen NIH, DOD, NJHF or other grant proposals for funding. We have had success (funded R01s, R21) in several areas and we continue to study p53 reactivators, Bmi-1 inhibitors, BMP-2 inhibitors, MTHFD2 inhibitors, and p38-ERK2 dual inhibitors with CINJ faculty. We also collaborate with Mito Biopharma in the area of metabolic diseases, with the Rutgers-Newark Medical School in a carbonic anhydrase program for autoimmune indications, and a plasmodium PKG program for malaria. We also collaborate with the Newark Camden based thyroid receptor agonist program. The group is composed of 6 professional chemists, and a graduate student and research interns from the school of pharmacy. This poster will cover two areas of study; the inhibition of Plasmodium G Kinase for the treatment of malaria and BMI-1 inhibitors for the treatment of glioblastoma.

Poster Abstracts

3. ASMIC - A Designer Isocyanide for Drug Discovery

J. Armando Lujan-Montelongo, Embarek Alwedi, Bhaskar R. Pitta, J. M. del Compo Ramirez, Allen Chao, and Fraser F. Fleming

Department of Chemistry, Drexel University, Philadelphia, PA.

ASMIC is an isocyanide building block that addresses the quest for an isocyanide - soon to be commercially available - capable of assembling tetrasubstituted isonitriles having diverse substituents. Extensive structural screening has identified a core structure in which an aromatic sulfide facilitates two sequential alkylations and a subsequent sulfur-lithium exchange-alkylation. A series of cyclic and acyclic isocyanides are readily prepared for subsequent use in multi-component reactions or heterocycle synthesis. The strategy provides a diverse array of tetrasubstituted isonitriles that are otherwise challenging to synthesize.

4. Inhibition of Adenylyl Cyclase 5, A Novel Therapeutic Modality to Reduce Infarct Size Even When Delivered After Coronary Artery Reperfusion

Jie Zhang[1], Daniel Levy[2], Thomas P. Richardson[2], Christopher Meenan[2], Dorothy E. Vatner[1 2], Stephen F. Vatner[1 2]

(1) Rutgers University - New Jersey Medical School, Newark, New Jersey, USA
(2) Vasade Biosciences, Inc., Barnegat Light, New Jersey, USA

Reducing myocardial infarct (MI) size in patients has been a major goal of the pharmaceutical industry over the past half century. However, It largely has been unsuccessful. One of the key reasons is that the drug must be delivered before coronary artery occlusion (CAO) or before CA reperfusion (CAR) to be successful. However, in the clinical setting CAR must precede other therapeutic interventions. It is also important for patients with CA disease and heart failure for the drug not to increase myocardial oxygen consumption. A novel candidate in the beta adrenergic blocker signaling pathway is inhibition of type 5 adenylyl cyclase (AC5). Our laboratory developed an AC5 knock out (KO) mouse, which protects against myocardial ischemia and oxidative stress (an important component of CAR injury) and also reduces beta adrenergic signaling and myocardial oxygen consumption.

Therefore, we developed a drug, C90, which inhibits AC5 and mimics the AC5 KO. Mouse cardiac membrane preparations were used to determine cAMP production. C90 reduced AC activity and cAMP, compared with vehicle, (12.9±1.86 vs. 14.2 ± 3.07 pmol/mg/min). However, in AC5 KO C90 no longer reduced cAMP in response to forskolin. C90 also demonstrated marked cardiac protection, even when delivered after CAR. Wild type mice were subjected to 30 min CAO followed by 24 hours CAR. C90 or vehicle was then administered at 5 min by intravenous (IV) administration at a dose of 0.06mg/kg. The area at risk was similar in all groups. However, MI size was reduced significantly, $p<0.05$, by 56% with C90 compared to vehicle (C90 infarct = 16±1.9% of the area at risk vs. vehicle infarct = 37±0.7% of the area at risk).

These properties make C90 an excellent candidate for clinical development, addressing several major challenges for effective pharmacological treatment of MI, since patients coming to the hospital with MI have no time to have drug delivered until after blood flow has been restored. An additional salutary feature of C90 is its ability to reduce AC activity and consequently beta adrenergic receptor signaling and myocardial oxygen consumption.

Poster Abstracts

5. Fox Chase Chemical Diversity Center, Inc.: Translating Basic Research Discoveries into Commercial Opportunities

Simon D. P. Baugh, Haiyan Bian, Tom A. Ford-Hutchinson, Katie Freeman, Tom Haimowitz, Jennifer Halgas, John Kulp, Brian J. Larsen, H. Marie Loughran, Mark E. McDonnell, Michael H. Parker, Jeff C. Pelletier, Camille Remeur, Robert J. Rosano, Richard W. Scott, Garry R. Smith, Eric D. Strobel, Colin M. Tice, Damian G. Weaver, Jay E. Wrobel, Hong Ye, Yan Zhang, Allen B. Reitz

Fox Chase Chemical Diversity Center, Inc.
3805 Old Easton Road, Doylestown, PA 18902
3700 Horizon Dr., King of Prussia, PA 19406

Fox Chase Chemical Diversity Center, Inc. (www.fc-cdci.com) provides medicinal chemistry, target validation, in vitro pharmacology and chemical biology support to investigators at universities, and non-profit research organizations and foundations. Our goal is to transition innovative biomedical research technologies into full-fledged drug discovery and development programs of study. In this poster we describe the services and capabilities offered by FCCDC to support the research community.

6. BUGS ON DRUGS; Biodegradation, Fate and Ecotoxicity of Pharmaceuticals and Personal Care Products (PPCPs)

Aamani Rupakula[1]*, Michelle Zeliph[1], Bing Hong[2], Shen Yu[2], Max M. Häggblom[1]#

(1) Department of Biochemistry and Microbiology and
(2) Department of Environmental Science, Rutgers, The State University of New Jersey, New Brunswick, NJ;
(3) Institute of Urban Environment, Chinese Academy of Sciences, Xiamen, China.
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Pharmaceuticals and personal care products (PPCPs) are emerging contaminants in river and estuarine ecosystems throughout the world. Wastewater treatment plant (WWTP) effluents are one of the main pathways for entry of PPCPs into watersheds where they can have adverse effects on the aquatic biota. Our overall goal is to determine the environmental fate and effects of PPCPs and their metabolites. We monitored a set of over 100 PPCP compounds in WWTP influent and effluent by liquid chromatography-mass spectrometry to assess their fate. Among the most abundant PPCPs in the sewage influent were the anti-inflammatory drugs aspirin, acetaminophen, ibuprofen, and diclofenac, which were selected for biodegradation studies.

The potential for biodegradation and transformation of these PPCPs was examined to better understand their fate in the environment and identify potentially problematic metabolites. To mimic different conditions in WWTP sludge, as well as river and estuarine environments, microcosms were established under sulfidogenic, methanogenic, and denitrifying redox conditions and dosed with acetaminophen, aspirin, diclofenac, or ibuprofen. The extent of biodegradation or transformation observed in the microcosms was dependent on both the redox conditions and the PPCP. Anaerobic degradation of aspirin and acetaminophen was observed under the three redox conditions tested, while diclofenac and ibuprofen were recalcitrant. The results of these experiments suggest that these compounds are degraded to various degrees by native microorganisms in WWTPs and river and estuarine sediments. Depending on the dominant redox condition of the sediment, certain PPCPs may be recalcitrant in the natural environment. Future experiments will focus on enriching and identifying the microbial community members involved in aspirin and acetaminophen biodegradation, as well as identifying metabolites and characterizing the biodegradation pathways.

Poster Abstracts

7. Avalanche Discovery Assistant

Vladyslav Kholodovych[1] and William J. Welsh[1 2]
[1]Rutgers, The State University of New Jersey; [2]Snowdon, Inc.

Snowdon, Inc. (snowdonpharma.com/), together with Rutgers University, announce the Avalanche Discovery Assistant computational tool that has been specifically designed to help biopharmaceutical companies generate drug leads leading to new intellectual property. Avalanche Discovery Assistant goes beyond traditional virtual screening tools by incorporating both shape and pharmacophoric feature-based comparison with 3D alignment between the query molecule and test compounds residing in chemical databases. Moreover, the Avalanche algorithm automatically incorporates the perspective of the target protein receptor during the process.

Avalanche Discovery Assistant excels at scaffold hopping, thereby finding new drug prospects whose structures may differ radically from the query. By incorporating molecular shape and pharmacophoric features with 3D alignment in the process, Avalanche Discovery Assistant enhances prospects in finding more uncommon hits that would be missed by traditional virtual screening methods. As an idea generator it also offers clues that enable medicinal chemists to discover new hits and leads with improved safety and bioactivity profiles and better prospects for patentability in drug discovery campaigns. Avalanche Discovery Assistant incorporates valuable searchable databases for insights into drug-like properties, mechanism of action, undesired toxicity, and commercial availability of potential leads.

Snowdon Inc. is a technology-driven company that specializes in the creation of computational tools and techniques for the life sciences including drug discovery and development, safety/toxicity assessment, and environmental/toxicological surveillance. The Company also engages in direct collaborative interactions with clients and partner companies, which include DeltaSoft, ChemDoodle, and Romark Laboratories. For further information or inquiries, contact info@snowdonpharma.com.

8. Repurposing Senicapoc For The Treatment Of Neuropathic Pain

Roland Staal[1], Ph.D., Andrew H. Berks[2], Ph.D., J.D.
[1]Alentis Pharma LLC, Metuchen, NJ; [2]Cittone and Chinta LLP, New York, NY

Neuropathic pain is a debilitating, chronic condition with a significant unmet need for safer and more effective treatment options. Recent studies have demonstrated that in addition to neurons, non-neuronal cells such as microglia contribute to the initiation and maintenance of allodynia in rodent models of neuropathic pain. It is believed that sedation, addiction, and other central nervous system side effects are mediated by the expression of drug targets by neurons in pain pathways, as well as other pathways such as the reward pathway. KCa3.1 is a potent regulator of various microglial responses to injury, including cytokine and nitric oxide release. Not only is KCa3.1 not expressed on neurons, it is only expressed by microglia in injured areas of the brain and spinal cord, further mitigating the chances for unwanted side effects.

We show that senicapoc readily enters the brain at concentrations similar to those used in clinical trials. Senicapoc is a potent, selective inhibitor of KCa3.1. It has been shown to to reducE pain responses in models of neuropathic pain without the side effects observed with gabapentin. Furthermore, screening in a multiple pain assays was suggestive of efficacy in models of other chronic and neuropathic pain indications. The safety profile of Senicapoc has also been demonstrated in the clinic. Senicapoc, which was originally developed for the treatment of sickle cell anemia, was evaluated in Phase 1, 2 and 3 clinical trials virtually without significant side effects. Thus, initial studies suggest that senicapoc may be a safe, potent inhibitor of KCa3.1 with efficacy in models of neuropathic pain. Future work will focus on identifying the pain indications which are most likely to respond to treatment with senicapoc, as well as identifying biomarkers to demonstrate target engagement in the clinic.

Poster Abstracts

9. Overcoming Formulation Challenges in the Era of Biotherapeutics

Herschel Rabitz,[1] Genyuan Li,[1] Xi Xing,[1] and William J. Welsh[2]
[1]Princeton University; [2]Rutgers, The State University of New Jersey

Opportunity: Global revenues in biopharmaceutical companies are being fueled by innovations in biotherapeutics, largely in oncology, immunology, and diabetes.
Challenge: Finding the optimal formulation conditions of aggregation-prone proteins in biotherapeutics.
Requirement: Formulations must contain a complex combination of buffers, excipients, surfactants, and solvent mixtures to temper the interactions between the protein molecules (e.g., mAbs).
Current Status: Formulation efforts in pharma are ad hoc and low-dimensional, i.e., "see how 1-2 solution variables affect protein stability and aggregation".
Risk: This limitation in the formulation stage creates a "choke point", leading to product delay or discontinuation.
Our Solution: The High-Dimensional Model Representation (HDMR) approach is a revolutionary data analysis tool that enables the formulation scientist to explore how all possible solution variables affect protein stability and aggregation simultaneously. HDMR builds an analytical expression between the Inputs "X" (solution variables: buffers, excipients, surfactants, solvent mixtures, etc.) and the Output "Y" (protein stability) by sampling various combinations and concentrations of the solution variables in a 384-well microarray format and measuring protein stability. The HDMR expansion $Y = \Sigma f(X)$ converges rapidly after a few terms to yield the Input-Output relationship.
HDMR requires only sparse sampling of the full range of solution variables, and scales well with variables that number in the 10s, 100s, or even 1000s. Counterintuitively, HDMR holds that working with more variables increases the likelihood of success. HDMR automatically ranks and quantifies the significance of each solution variable individually and cooperatively, and pinpoints regions of high and low protein stability. HDMR reveals valuable insights, such as the optimal formulation using any number of solution variables and the smallest number of solution variables that assure product quality specifications. HDMR is extensible to many other applications along the drug discovery & development pipelines. This poster will present results from a multi-year collaboration with a top-10 pharmaceutical company. For further information or inquiries, contact welshwj@rwjms.rutgers.edu.

10. CCR1 Antagonists Demonstrate in vitro Efficacy for Glioblastoma

James Merritt, Ph D.; Molly Gill, M.S.; Dhruvishaben Patel, M.S.; Poornema Ramasunduram, M.S.; Yuriko Root, M.S.; Joe-Louis Yarfi, M.S.; Salvatore Coniglio, Ph.D.
Kean University

Chemotactic Cytokine Receptor 1 (CCR1) belongs to a large family of chemokine receptors that interact with specific chemotactic ligands to mediate inflammatory leukocyte trafficking. Ligands of CCR1 include CCL3, CCL5 and myeloid progenitor inhibitory factor-1 (MPIF-1). We have observed that CCR1 ligands are upregulated in glioblastoma and tumor associated macrophages/microglia. Glioblastomas are aggressive astrocytic tumors that reproduce rapidly and are aggressively malignant. The ability of glioblastoma tumor cells to infiltrate surrounding brain tissue limits effectiveness of current treatments. We have demonstrated that small molecule, CCR1 antagonists inhibit the ability of microglia to stimulate the invasion of a glioblastoma cell line.

Poster Abstracts

11. Lilly's Open Innovation Drug Discovery (OIDD) Program - For Scientists, By Scientists

David Bleakman[1], Kurt Rasmussen[2]

[1] *Neuroscience Research, Eli Lilly and Company, 430 East 29th St., 12th Floor, New York, NY*

[2] *Neuroscience Research, Eli Lilly and Company, Lilly Corporate Center, Indianapolis, IN*

Through the OIDD program, we engage external investigators in a hypothesis-driven approach to early drug discovery. Investigators gain access to the same tools and expertise available to our scientists to design, test, and make new molecules while at the same time retaining complete control of their data and Intellectual Property. In addition, investigators can use our molecules to test their own biological hypotheses. Information about the capabilities offered, how the program differentiates from others in the industry, how data and Intellectual Property is protected, and how to get started are just a few of the key areas that will be covered.

12. Antiviral Agents Targeting Poxviruses Through Inhibition of the Function of Processivity Factors

Michael H. Parker[1]*, Simon D. P. Baugh[1], Eric D. Strobel[1], Manunya Nuth[2], Hancheng Guan[2], Stuart N. Isaacs[3], Allen B. Reitz[1], Richard W. Scott[1], and Robert P. Ricciardi[2]

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In poxviruses such as vaccinia virus and molluscum contagiosum virus, the processivity factors A20 and D4 are proteins required for viral replication. A20 and D4 associate to form a D4-A20 heterodimer that interacts with the viral DNA polymerase to enable it to efficiently synthesize extended strands of DNA. Disruption of this interaction is therefore a potential mechanism for therapeutic antiviral agents. Because processivity factors have a high degree of variability between different viruses, targeting the D4-A20 heterodimer is expected to be selective in regard to other types of viruses. We have designed and synthesized small molecules that target this interaction and exhibit in vitro antiprocessivity activity, antiviral activity in cells, and protection against infection in a mouse model.

13. The Role of Microbiota-Derived Small Molecules in the Etiology of Crohn's Disease

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Crohn's disease (CD), which is characterized by chronic inflammation of the gastrointestinal tract, is a complex disorder in which aberrant immune responses to the gut microbiota is a key contributor to pathogenesis.[1] The composition of the human gut microbiome in CD patients has been long known to be distinct from that of healthy subjects, yet very little is understood about the functional consequences of this distinction.[2] The CD microbiome may harbor unique pro-inflammatory features that elicit or exacerbate inflammation, or anti-inflammatory features that help members of the microbiome survive in the hostile inflammatory environment. Very few studies have aimed to discover such features, or explore their chemical and biological properties.

Here, we hypothesized that the CD microbiome produces a different suite of small molecules than that of healthy subjects, and that these molecules are functionally involved in the causation or response to the disease. By using a novel computational algorithm, we identified a subset of small molecule biosynthetic gene clusters that are statistically significantly enriched in the gut microbiome of CD patients, none of which has been previously characterized. **Continued Next Page.**

Poster Abstracts

Through a synthetic biology strategy, where gut microbiome-derived gene clusters are cloned and expressed in an engineered heterologous host, we obtained three members of these molecules. HPLC-HRMS/MS and NMR experiments revealed their structures as novel modified peptides, and efforts to elucidate their biological activities in the context of Crohn's Disease are currently ongoing. In summary, we combined computational and synthetic biology approaches to discover a set of unique and previously-undescribed small molecules that are significantly enriched in the microbiome of CD patients.

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14. Development of an EBNA1 Inhibitor for the Treatment of EBV-Positive Cancer

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BACKGROUND: New therapeutic approaches are needed for cancers associated with Epstein-Barr Virus (EBV). EBV is etiologically associated with a diverse collection of malignancies, including nasopharyngeal carcinoma (NPC), Burkitt's lymphoma, Hodgkin's and non-Hodgkin's lymphomas, and subtypes of gastric carcinoma. Indeed, EBV is responsible for over 200,000 cases worldwide. The World Health Organization has classified EBV as a human class I carcinogen. Currently, no pharmaceutical-based therapies exist that selectively target EBV associated cancers. EBV, in its latent oncogenic form, is dependent on the continuous expression of Epstein-Barr Nuclear Antigen 1 (EBNA1), a multifunctional dimeric protein critical for viral genome replication, mitotic segregation, and viral gene expression. EBNA1 is unique with no structural analogs in the human proteome.

METHODS: The aim of this program is to advance the development of a New Chemical Entity (NCE) for latent infection of Epstein-Barr Virus (EBV) to treat EBV-associated cancer. We used structure-based drug design (70+ co-crystal structures) and medicinal chemistry methods (2500+ compounds synthesized) to identify and develop a small molecule clinical candidate that selectively inhibits the DNA-binding activity of EBNA1 and inhibits EBV-associated tumor cell growth in four different mouse models of EBV-associated cancer.

RESULTS: The clinical candidate inhibits EBNA1 function with nanomolar potency in biochemical assays and low micromolar activity in several cell-based assays. We demonstrate that EBNA1 inhibitors provide protection in 4 different xenograft models of EBV-driven tumor growth, including lymphoblastic B-cell lymphoma and patient-derived xenografts for nasopharyngeal carcinoma. Furthermore, RNA analysis experiments (by EBER-ISH and Nanostring-based technology) confirm in vivo target engagement by the elimination of EBV in treated tumor tissue. EBNA1 inhibitors are selective, showing little to no activity in an EBV-negative xenograft experiment.

The clinical candidate has met industry-accepted criteria for drug suitability including in vitro ADME: physicochemical properties, metabolic stability, Cyp inhibition and induction, hERG, Ames genotoxicity and selectivity in broad-based screens. Pharmacokinetic studies indicate that the candidate is orally bioavailable, attaining high plasma levels with a relatively linear dose-exposure response in mouse, rat and dog. In 28-day repeat dose toxicity studies, we observe no toxicology findings that would preclude further development. The candidate exhibits a favorable predicted therapeutic index, possibly reflecting the lack of an endogenous target in uninfected cells. We have also performed salt selection, polymorph analysis and forced degradation studies and optimized the process chemistry for the synthesis of kilogram quantities of the API. **Continued Next Page.**

Poster Abstracts

CONCLUSIONS: IND-enabling studies including safety pharmacology and toxicology and GMP manufacturing have begun with a projected IND filing in H1 2018. A First-In-Human clinical trial could commence in 2018 depending on available funding.

15. Synthesis of a cis-Decalin Inhibitor of Rad52: Inducing Synthetic Lethality in BRCA Deficient Cancers

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Mutations in the BRCA1 and BCRA2 tumor suppressor genes led to an increased risk of breast, ovarian, prostate, colon, and pancreatic cancers. In 2011, Feng et al. determined that selectively targeting RAD52 in BRCA deficient cells led to selective synthetic lethality due to complete inhibition of both homologous recombinant repair pathways. A virtual screen of the ZINC database was used to identify possible small molecule inhibitors of RAD52. A cis-decalin based natural product, 3,4-dihydroxyclerodan-13E-en-15-oic acid, showed promise.

Further investigation with a DNA pull down assay confirm both the affinity and selectivity (over RAD51) of this compound for RAD52. No longer commercially available, presented here is the progress towards a diastereoselective total synthesis of this ground breaking compound. The synthetic strategy began with the optimization of classic steroid synthetic techniques. Then, the thermodynamically disfavored cis-decalin is introduce with a Crabtree reduction. The molecule can then completed by a series of carefully timed oxidation and reduction reactions, which utilizes the thermodynamic preference for equatorial substitutions in a cyclohexane to direct the stereochemical outcome. The first 10 steps of the proposed 16 step synthesis have been completed with a 2.5% over yield.

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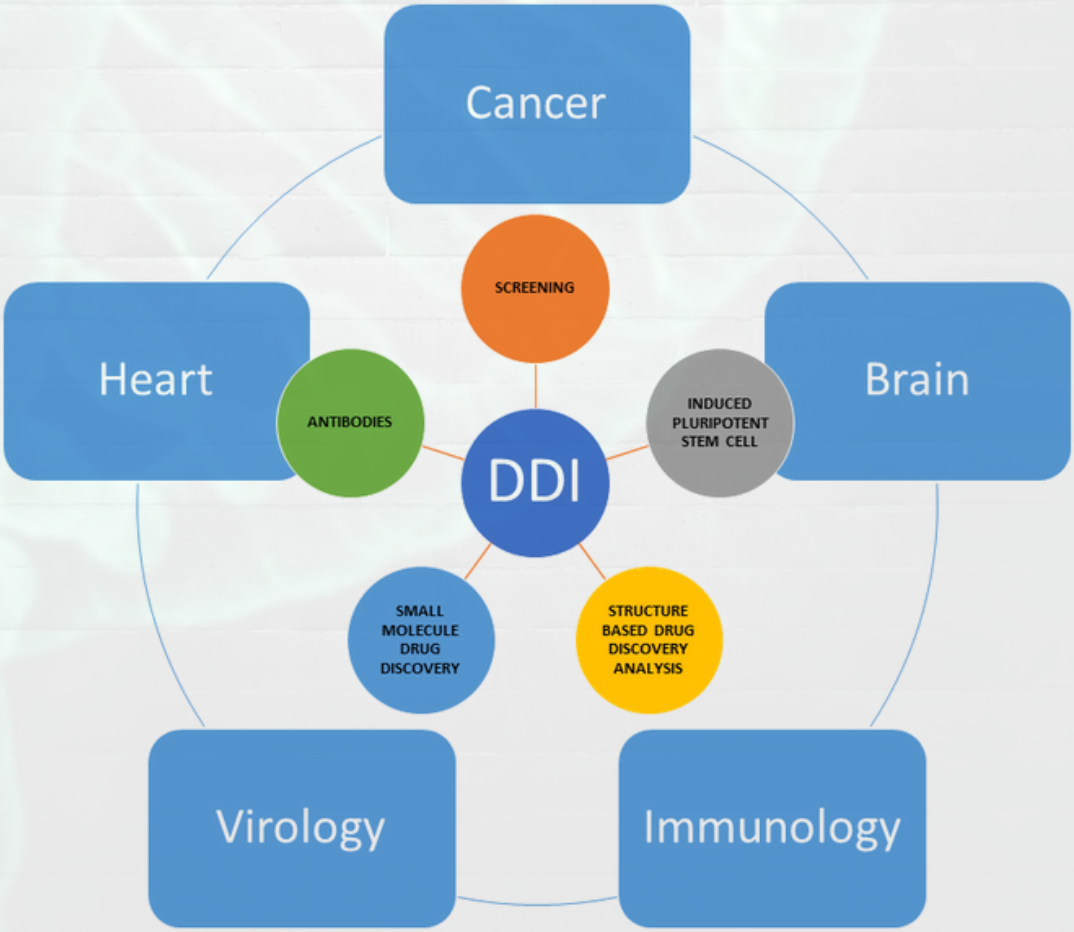

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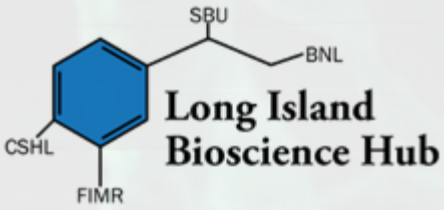

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