ACS chemical biology

INTRODUCING OUR AUTHORS

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Bonnie Baxter

Image courtesy of Vince Sullivan.

Current position: Research Assistant Professor, Dept. of Pediatrics/Division of Infectious Diseases, University of Rochester Medical Center, Rochester, NY, working with Professor Damian Krysan

Education: Butler University, B.A. in Psychology, 1990; University of Wisconsin, Ph.D. in Biomolecular Chemistry, 1997

Nonscientific interests: Parenting, gardening, cooking, living with multiple sclerosis

Our research focuses on exploiting large chemical and genetic libraries to uncover new methods of antifungal drug discovery, and to learn about the genetics and mechanisms of critically important but poorly understood pathogenic fungi such as *Cryptococcus neoformans* and *Candida albicans*. These organisms and their close relatives cause untold suffering and countless deaths, particularly among immunocompromised people around the world. These high levels of morbidity and mortality are largely because of the very small number of drugs available to fight such infections. We hope that our research will contribute to understanding these organisms more fully and being able to fight them more effectively. My previous experience with the genetics and biochemistry of the model organism *Saccharomyces cerevisiae* and the vast community of researchers and body of accumulated understanding of this model system contribute significantly to this work. (Read Baxter's article, DOI: 10.1021/cb100399x)

Renzo Corzano

Image courtesy of Cindy Zer.

Current position: City of Hope Beckman Research Institute, Department of Molecular Medicine, Ph.D. candidate in the laboratory of Dr. John C. Williams

Education: University of California, Riverside, B.S. in Biochemistry, 2008

Nonscientific interests: Hiking, soccer, chess, music, movies, the beach, and making my labmates laugh

My research in Dr. Williams' laboratory is focused on inhibition of the transcription factor STAT3. Many types of cancers depend on constitutively activated STAT3 for proliferation and survival. STAT3 inhibition leads to growth arrest and apoptosis in cancer cells and is, therefore, an ideal target for cancer therapy. I combine X-ray crystallography, mass spectrometry, fragment-based drug design, and other biophysical techniques to identify a specific small-molecule STAT3 inhibitor. My long-term goals after obtaining my Ph.D. are to pursue a postdoctoral or industry position in the field of drug discovery. Our paper shows that cysteine 468 in STAT3 is susceptible to alkylation by compound C48, resulting in DNA binding inhibition by steric hindrance. We also show that STATTIC (a STAT3 inhibitor) is also an alkylator. These results indicate that reactive cysteines can be exploited for therapeutic purposes. (Read Corzano's article, DOI: 10.1021/cb100253e)

Shan Gao

Image courtesy of Dr. Yatao Liu.

Current position: Massachusetts General Hospital, Center for Engineering in Medicine, Postdoctoral Fellow with Prof. Martin L. Yarmush

Education: East China University of Science and Technology, Shanghai, China, B.S. and M.S. in Chemical Engineering, 2000 and 2003; Columbia University, Ph.D. in Chemical Engineering with Prof. Scott Banta, 2009

Nonscientific interests: Traveling, photography, cooking, reading and writing

As a graduate researcher in the Department of Chemical Engineering at Columbia University, my work focused on engineering delivery vehicles to shuttle proteins and nucleic acids into brain cells for the treatment of central nervous system disorders. Our delivery vehicles use cell-penetrating peptides (CPPs), a cationic amino acid sequence known to cross cell membranes with high efficiency. To optimize CPPs for our application, we established a plasmid display system for screening novel CPPs with desired properties from combinatorial peptide libraries. By using this display and screening platform, described in this article, we identified an unusual peptide that exhibited a cell-penetrating phenotype but did not have pronounced positive charges like conventional CPPs. Currently, I am a postdoctoral fellow at the Center for Engineering in Medicine at Massachusetts General Hospital where we have developed a

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complementary technology to study drug delivery and the host response by creating microchips that contain fluorescent reporter cells as diagnostic sensors of inflammation. (Read Gao's article, DOI: 10.1021/cb100423u)

Stamatios Liokatis

Image courtesy of Stamatios Liokatis.

Current position: Leibniz Institute for Molecular Pharmacology, Department of NMR-assisted Structural Biology, Postdoctoral Researcher with Philipp Selenko, 2008−present

Education: University of Ioannina, Greece, B.S. in Chemistry, 1999; University of Ioannina, Greece, Master in Biochemistry with Marilena Lekka, 2002; University of Ioannina, Greece, Ph.D. in Biochemistry with Anastasia Politou, 2008

Nonscientific interests: Music, movies

My research field is chromatin biology. During my Ph.D. I studied the structural and functional properties of a chromatin-binding domain. Currently, at the FMP-Berlin, I am investigating the mechanistic properties of histone-modifiyng enzymes using nuclear magnetic resonance (NMR) spectroscopy. This research focuses on the most prevalent post-translational protein modifications (phosphorylation, acetylation). In this paper, we report tools to map lysine acetylation on degenerate protein sequences, using NMR spectroscopy. (Read Liokatis' article, DOI: 10.1021/cb1003866)

Kathrin Schirner

Image courtesy of Kathrin Schirner.

Current position: Harvard Medical School, Department of Microbiology and Molecular Genetics, DFG Postdoctoral Fellow with Suzanne Walker

Education: Eberhard-Karls-University Tübingen, Germany, Diploma in Biology with Wolfgang Wohlleben, 2005; Newcastle University, U.K., Ph.D. in Microbiology with Jeff Errington, 2009

Nonscientific interests: Playing the violin, traveling, enjoying life

I am generally interested in deciphering fundamental processes of bacterial cell biology. My postdoctoral research is focused on studying how wall teichoic acids, crucial components of the cell wall of Gram-positive bacteria, are transported across the cell membrane by an ABC transporter. It is a question of general interest, because other bacterial polymers such as capsules and lipopolysaccharides are transported by similar systems. Additionally, it is simply an intriguing problem: how can a large charged polymeric molecule be moved across a membrane by a small transporter? To begin elucidating the transport mechanism, we present here studies on the specificity of the transporter for different substrates in live bacteria by heterologous complementation and the use of a highly specific small molecule inhibitor. (Read Schirner's article, DOI: 10.1021/cb100390w)

Jessica Slack

Image courtesy of Christin Gavin.

Current position: The Scripps Research Institute, Department of Chemistry, Postdoctoral Fellow with Paul R. Thompson

Education: Smith College, B.A. in Biochemistry, 2006; University of South Carolina, Ph.D. in Biochemistry with Paul R. Thompson, 2010

Nonscientific interests: Beer brewing, cooking unusual things, skydiving and kickball

My research interests are focused on the elucidation of Protein Arginine Deiminase 4 function, activity and activation dynamics. Enormous effort has been made toward understanding the physiological roles of this protein modifying enzyme, due to the increasing evidence linking dysregulated PAD activity to the incidence and severity of rheumatiod arthritis (RA) and other human diseases, such as cancer and colitis. In my study, we have developed and employ a series of activity-based protein profiling probes to study the dynamics of PAD4 expression, activity, and function, in hopes of obtaining a better understanding of how this enzyme plays a role in these important human diseases. (Read Slack's article, DOI: 10.1021/cb1003515)

Sydney Stoops

Image courtesy of Sydney Stoops.

Current position: Vanderbilt University, Department of Pharmacology, Ph.D. Candidate with Prof. Craig W. Lindsley

Education: Miami University, B.A. Microbiology, minor in Molecular Biology, 2007

Nonscientific interests: Traveling, baking, exercise, fashion, watching college basketball and football

My research focuses on the optimization of a high-throughput screening hit shown to upregulate E-cadherin protein expression in a colorectal cancer cell line. E-Cadherin is a transmembrane protein that maintains intercellular contacts and cellular polarity in epithelial tissues. The down-regulation of E-cadherin is thought to aid in the induction of epithelial-to-

mesenchymal transition (EMT) resulting in an increased potential for invasion into the surrounding tissues. My experiments aim to develop structure−activity relationship around the lead screening hit in order to improve E-cadherin restoration as well as identifying the molecular target and mechanism by which the compounds are acting in the cell. Such data will aid in understanding the role of E-cadherin in tumor invasion and metastasis as well as identify potential therapeutic targets. (Read Stoops' article, DOI: 10.1021/cb100305h)

Kiwamu Takemoto

Image courtesy of Kiwamu Takemoto.

Current position: Yokohama City University, Department of Physiology, Assistant Professor

Education: Osaka University, B.S. in Biology, 1997; Osaka University, Ph. D. in Medicine, 2004

Nonscientific interests: Football

My research here at Yokohama City University is focusing on the decoding and controlling of brain information in the hippocampus. In the brain hippocampus, many neuronal cells make handshakes, called synapses, that are functional and minimum units of signal transduction between neurons. Although controlling methods for neuronal cells, such as channel rhodopsin-2 are available, controlling of single synaptic activity is difficult to realize by conventional methods. Using eosin-based CALI method, I'm now trying to develop a loss of function technology of a single synaptic function with local laser irradiation. This technique will become a promising tool for decoding brain information in living animals. (Read Takemoto's article, DOI: 10.1021/cb100431e)

Mengmeng Zhang

Image courtesy of Xi Chen.

Current position: University of Texas at Austin, Department of Chemistry and Biochemistry, Ph.D. candidate with Prof. Yan Zhang, 2008−present

Education: Shanghai Jiao Tong University, B.E. in Bioengineering, 2006; Clemson University, M.S. in Biological Sciences, 2008

Nonscientific interests: Traveling, movies, music, swimming

My research interests have been focused on a human phosphatase that silences the expression of neuronal genes and is, therefore, a novel target for neuroregeneration. This protein, named small CTD phosphatase (Scp), dephosphorylates the phosphorylated Ser5 of the C-terminal domain (CTD) of eukaryotic RNA polymerase II. I have used X-ray crystallography and enzyme kinetics to capture the phosphoaspartyl intermediate of the phosphoryl transfer catalyzed by Scp, providing evidence for its proposed catalytic mechanism. Moreover, modifications of the CTD (termed the CTD code) are essential for the function of RNA polymerase II; therefore how the CTD code is deciphered has become a very interesting topic. Small molecule inhibitors which target Scp may prove useful in promoting neuronal differentiation. In this paper, we have successfully identified a lead compound for Scp with very good selectivity using high-throughput screening and kinetic study. Cross-inhibition toward other phosphatases, a bottleneck for phosphatase inhibitor study, has been overcome for this compound. The inhibition mechanism and compound selectivity were interpreted beautifully with the complex structure of Scp with this compound. (Read Zhang's article, DOI: 10.1021/cb100357t)