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INTRODUCING OUR AUTHORS

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Ahmet Altun

Image courtesy of Ahmet Altun.

Current position: Associate Professor at Fatih University, Department of Physics, Istanbul, Turkey

Education: Dokuz Eylul University, Turkey, B.S. in Physics, 1996; Fatih University, Turkey, M.S. in Physics, 1999; Institute of Technology, Gebze, Turkey, Ph.D. in Physics, 2003; Max-Planck-Institut für Kohlenforschung, Germany, Postdoctoral Fellow with Prof. Dr. Walter Thiel, 2006; Emory University, U.S.A., Postdoctoral Fellow with Profs. Dr. Keiji Morokuma and Shozo Yokoyama, 2010

Nonscientific interests: Music, traveling, movies, playing with my kids

My research interests include quantum mechanical (QM) and hybrid quantum mechanical/molecular mechanical (QM/MM) calculations on the molecules *in vacuo* and in their native protein/solvent media for determining their geometries, electronic structures, spectral parameters, reaction mechanisms, photochemical characteristics, structure−bioactivity relationships, *etc.* I am also experienced in synthesis and thermal/spectral characterization of transition metal complexes. I am currently active in theoretically revealing and characterizing the catalytic species and reaction mechanisms of cytochrome P450 enzymes and the mechanisms of spectral tuning in visual pigments that involve the reasoning under the protein-specific color detection of retinal in the full UV−vis and near IR regions with the aid of QM/MM calculations. (Read Altun's article, DOI: 10.1021/cb200100f)

Shiva Angala

Image courtesy of Shiva Angala.

Current position: Graduate student pursuing Ph.D. at Colorado State University under the supervision of Dr. Delphi Chatterjee at Mycobacteria Research Laboratory, Department of Microbiology, Immunology and Pathology

Education: B.S. in Microbiology, Genetics and Chemistry at Osmania University, Hyderabad, India, 2000; M.Sc. in Biotechnology at Osmania University, Hyderabad, India, 2002

Nonscientific interests: Music, Cricket, long road trips with family and friends, social service

I have developed strong aptitude for genetics, molecular biology, genetic engineering and microbiology. My Ph.D. research started with high-throughput screening of drug candidate compounds using a microtiter plate and whole cell Alamar Blue assay. I have successfully screened nearly 3000 compounds for *Mycobacterium tuberculosis* growth inhibition. A major part of my research is focused on development of cell free enzymatic assays for the membrane bound Arabinosyltransferases that are involved in the cell wall biosynthesis of *M. tuberculosis*. In the work described, we solubilized and purified arabinosyltransferase C (AftC) and reconstituted it into functionally active AftC proteoliposomes. We developed a cell free arabinosyltransferase assay using AftC proteoliposomes and assessed varied synthetic donors and acceptor analogs for its transferase activity. This work involves extensive analytical approach to the analysis of enzymatic product. (Read Angala's article, DOI: 10.1021/cb200091m)

Angeles Canales

Image courtesy of Gabriel Deseff.

Current position: Universidad Complutense of Madrid, Department of Organic Chemistry, Associate Researcher (Ramón & Cajal postdoctoral contract) with M. Luz López-Rodríguez

Education: Universidad Autónoma of Madrid, B.S. in Chemistry, 2000; Centro Investigaciones Biológicas (CSIC), Ph.D. in Chemistry with Jesús Jiménez-Barbero, 2005; Postdoctoral Researcher, Rovi Pharmaceuticals, 2006−2009

Nonscientific interests: Hiking and mountain sports

My research is focused on molecular recognition studies using NMR and molecular modeling protocols. My interest arose from my Ph.D. work on carbohydrate recognition and has been evolving toward drug design. At present, I am in the middle of three different projects, targeting MGL enzyme within the lab of Prof. M. Luz López-Rodríguez, exploring the interactions of glycosylaminoglycans with fibroblast growth factors and their receptors, collaborating with Prof. J. Jiménez-Barbero and understanding the interactions of tubulin with microtubule stabilizing agents (MTAs), in collaboration with Dr. J. F. Díaz. In this paper, we have carried out a systematic study to characterize the interaction of two MTAs with tubulin in its different aggregation states. This work sheds light on the mechanism by which these antitumoral drugs exert their function showing a dual role of the drugs since not only stabilize microtubules once are formed but also promote microtubule assembly. (Read Canales' article, DOI: 10.1021/cb200099u)

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Anshuman Dixit


Image courtesy of Anshuman Dixit.

Current position: University of Kansas, Bioinformatics core facility, Postdoctoral Researcher with Gerald H. Lushington since May 2010

Education: B. Pharm. in Pharmaceutical Sciences, Dept. of Pharmaceutical Sciences, Dr. Hari Singh Gour University, Sagar, India, 1997; M. Pharm. in Pharmaceutical Chemistry with Prof. D. V. Kohli, Dept. of Pharmaceutical Sciences, Dr. Hari Singh Gour University, Sagar, India, 1999; Ph.D. in Medicinal Chemistry and Cheminformatics with Dr. Anil K. Saxena, Medicinal Chemistry Division, Central Drug Research Institute, Lucknow, India, 2007; Postdoctoral Researcher with Dr. Gennady M. Verkhivker, University of Kansas, USA, 2007−2010

Nonscientific interests: Chess, music, traveling and current affairs

My postdoctoral research involved computational modeling studies of two important protein families: protein kinases and HSP90. We studied the functional role of kinase mutations in altering protein kinase structure, dynamics and stability and found that the mutants tend to destabilize the inactive kinase structures. We also studied structural transition of ABL and EGFR kinases computationally and proposed a multi stage mechanistic model of protein kinase activation. The Hsp90-family of proteins are molecular chaperones that have important role in facilitating post-translational maturation of various proteins. Our studies on HSP90 are focused on computational modeling of the energetic and structural changes, upon interaction with other small/macro molecules. These studies have helped in elucidating important interactions of novobiocin at the C-terminal binding site of human HSP90 and can further help in design of specific modulators for these pharmaceutically important proteins. (Read Dixit's article, DOI: 10.1021/cb200052x)

Jennifer Fishovitz


Image courtesy of Jennifer Fishovitz.

Current position: University of Notre Dame, Department of Chemistry and Biochemistry, Postdoctoral Researcher with Prof. Shahriar Mobashery

Education: Gannon University, B.S. in Chemistry, 2005; Case Western Reserve University, Ph.D. in Chemistry with Prof. Irene Lee, 2011

Nonscientific interests: Reading, music, movies

My graduate work focused on two ATP-dependent mitochondrial proteases that have been implicated in the maintenance of mitochondrial integrity, Lon and ClpXP, and the design of peptide-based substrates and inhibitors specific to each based on their different substrate specificities. The most exciting part of my research was to be able to use these enzyme-specific compounds to monitor the ATP-dependent peptidase activity of Lon in isolated mitochondria. While at this time, the results are mostly qualitative, they provide a foundation for the development of diagnostic tools that can be used to identify physiological protein targets. Furthermore, this information will be valuable for future drug design for the treatment of diseases associated with a decline in mitochondrial integrity. (Read Fishovitz's article, DOI: 10.1021/cb100408w)

Min Li


Image courtesy of Min Li.

Current position: Research Associate with Dr. Carolyn Suzuki, University of Medicine and Dentistry of New Jersey- New Jersey Medical School (UMDNJ-NJMS), Department of Biochemistry and Molecular Biology

Education: Tongji Medical College of Huazhong University, Hubei, China, M. D. in Clinical Medicine, 1998; Ph.D. in Department of Obstetrics and Gynecology with Prof. Yongyu Sun, 2004; University of Medicine and Dentistry of New Jersey, Department of Cell Biology and Molecular Medicine, Department of Radiation Research, Postdoctoral Researcher with Prof. Dorothy Vatner and Prof. Edouard I. Azzam, 2006 −2010

Nonscientific interests: Music, reading, movies, sports, cooking and traveling

My Ph.D. research focused on polycystic ovary syndrome (PCOS) with insulin resistance and its relationship between obesity and hyperandrogenism. As a postdoctoral fellow in Dr. Dorothy Vatner's laboratory, my work addressed cardiac disease biogenesis and treatment employing molecular biology and cell biology techniques, and most specifically on cell cycle related kinase (CCRK). As a postdoctoral researcher in Dr. Edouard I. Azzam's group, I studied the effect of radiation on mitochondrial protein import, mitochondrial aconitase activity and oxidative modification of proteins. As a Research Associate with Dr. Carolyn Suzuki, we are exploring the regulation of mitochondrial ATP-dependent proteases in mitochondrial protein and DNA quality control. In this work, we report DBN93 can enter the mitochondrion to inhibit the Lon protease in the matrix. (Read Li's article, DOI: 10.1021/cb100408w)

Ryan Marcheschi


Image cortesy of Dr. Rachel L. Britt.

Current position: University of California-Los Angeles, Department of Biomolecular and Chemical Engineering, Postdoctoral Employee, advisor Prof. James C. Liao

Education: University of Wisconsin-Madison, Department of Biochemistry, Ph. D. Biochemistry, advisor Prof. Samuel E. Butcher, 2009; Iowa State University, B.S. Genetics, academic advisor Prof. Sheldon S. Shen, research advisor Prof. Kristen M. Johansen, 2004

Nonscientific interests: Watching college football, gardening, attending orchestral performances, recreational hiking, playing trivia games, reading classic literature, going to local farmers' markets, drinking fine scotch

My graduate research focused on the characterization of translational frameshifting in HIV. An RNA stem-loop located at the frameshift site is used to program a (−1) nucleotide shift in the reading frame during translation. In this study, I present the structural characterization of a molecular complex between DB213, a HIV frameshifting stimulator that decreases viral replication, and the HIV-1 frameshift-site RNA. DB213 stabilizes the RNA and binds to a primary site located in the stem-loop that is likely present when frameshifting occurs. DB213 binding alters the conformation of the RNA, providing a potential explanation for its effect on frameshifting. This study provides a useful molecular scaffold for the development of compounds that specifically target the HIV-1 frameshift site RNA and thereby affect viral replication. (Read Marcheschi's article, DOI: 10.1021/cb200082d)

Laura B. Peterson

Image courtesy of Jessica A. Hall.

Education: The University of Colorado at Colorado Springs, B.S. Chemistry, 2007; The University of Kansas, Ph.D. Candidate in Medicinal Chemistry, Research Advisor: Brian S. J. Blagg

Nonscientific interests: Running, cooking, billiards, and coffee

My research at The University of Kansas is focused on the design and evaluation of heat shock protein 90 (Hsp90) inhibitors. Hsp90 is an essential molecular chaperone that plays a key role in various disease states, including cancer and neurodegenerative diseases. One class of Hsp90 inhibitors that bind to the Hsp90 C-terminal domain show promise and improved properties over other known inhibitory classes. Accordingly, elucidation of the Hsp90 C-terminal inhibitor binding site, which has been difficult to elucidate by other means, is extremely important for the future development of this promising class of Hsp90 inhibitors. (Read Peterson's article, DOI: 10.1021/cb200052x)

Jian Zhang

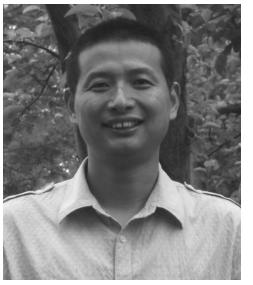

Image courtesy of Jian Zhang.

Current position: Research Scientist of ADA Technologies, Inc.

Education: Soochow University, B.S. in Chemistry, 1998; Shanghai Institute of Organic Chemistry, Ph.D. in Organic Chemistry, 2004; Colorado State University, Department of Microbiology, Immunology and Pathology, Postdoctoral Fellow with Prof. Delphi Chatterjee, 2004−2009

Nonscientific interests: Sports, fishing, traveling

My postdoctoral work at Colorado State University (CSU) focused on mycobacterial cell-wall carbohydrate biosynthesis, including the studies on mycobacterial GT-C membrane protein expression, purification, and glycosyltransferase function that are reported in this article. I worked with other colleagues at CSU to invent a novel proteoliposome system that can well retain arabinosyltransferase activity of AftC, a tough protein that has never been "living" in the environment absent of membranes. In 2010, I moved to ADA Technologies, Inc. and continue conducting carbohydrate research and developing glycotechnologies. Carbohydrate microarray, a unique technology to explore carbohydrate−protein interactions, has been my research focus here. (Read Zhang's article, DOI: 10.1021/cb200091m)