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Introducing Our Authors

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VIDUSHI ABROL

Image courtesy of Abhimanyu Abrol.

Education: B.Tech. Biotechnology and M.Tech. Biotechnology, Lovely Professional University (Jalandhar), Assistant Professor in C.T. Group of Institutes (Jalandhar)

Current Position: Ph.D. Scholar, School of Biotechnology, SMVDU, Katra (Jammu); Project Fellow, CSIR-Indian Institute of Integrative Medicine (Jammu), Advisors: Dr. Sundeep Jaglan and Dr. Sharada. M. Potukuchi

Nonscientific Interests: Reading fiction, aerobics, listening to music, driving, playing chess

My current research interests are chemical mutagenesis and isolation of secondary metabolites from important fungi and their bioactive potential. This strategy has been recently introduced to fungi, *i.e.*, a mutation-based mutagenesis strategy for the discovery of novel bioactive compounds from silent pathways of fungal secondary metabolites. By using chemical mutagenesis, we identified a new array of molecules and enhanced the yield of important metabolites, which were not produced by the fungi in normal media conditions. (Read Vidushi's article DOI: 10.1021/acschembio.7b00875.)

STEVEN M. ADELMUND

Image courtesy of Gabrielle Benuska.

Education: Washington State University, B.S. Chemical Engineering, 2008; Louisiana State University in Shreveport, M.S. Biological Sciences, 2014, Advisor: Dr. Elahe Mahdavian; University of Washington, M.S. Chemical Engineering, 2017, Advisor: Dr. Cole DeForest

Current Position: Ph.D. Student, University of Washington, Department of Chemical Engineering; Advisor: Dr. Cole DeForest

Nonscientific Interests: Running, hiking, gardening, raising chickens, and reading

My research operates at the interface of chemistry and biology, where I am applying bioorthogonal and photochemistries to establish tools uniquely capable of sampling the heterogeneous and dynamic nature of biology. Using a photocaged noncanonical amino acid, I have created a technique to label newly synthesized cellular proteins selectively at user-defined points in time and space for isolation and downstream proteomic analysis. I expect this tool to facilitate an enhanced understanding of biology by shedding light on the 4D proteomic changes that accompany disease and development. Combining this knowledge with the aforementioned chemistries, I am also interested in engineering next-generation biomaterials that recapitulate native biological complexity. These advances hold promise for the development of diagnostic tools and treatments for disease, as well as toward the continued advancement of variegated biomaterials for regenerative medicine applications. (Read Steven's article DOI: 10.1021/acschembio.7b01023.)

GLORIA ANDOLINA

Image courtesy of Gloria Andolina.

Education: Università degli Studi di Milano, Italy, B.Sc. Industrial Chemistry, 2009; M.Sc. Industrial Chemistry and Management, 2011, Advisor: Prof. Emanuela Licandro; University of Zurich, Switzerland, Ph.D. Chemistry (Biological Chemistry), Advisor: Prof. John A. Robinson

Current Position: Postdoctoral Fellow, University of Hong Kong, Hong Kong, Department of Chemistry, Advisor: Prof. Xuechen Li

Nonscientific Interests: Theater, opera, hiking, traveling, and reading

My Ph.D. research focused on gaining a better understanding of the interaction of a new class of antibacterial peptidomimetic (AMP) with the outer membrane protein LptD. The target protein is responsible for the transport of LPS to the surface in Gram-negative bacteria, and the novel AMP inhibits the biosynthesis of the outer membrane in *P. aeruginosa*. Our paper highlights the unicity of the LptD structure in *P. aeruginosa*

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and describes the work that was necessary to identify the binding site of the AMPs, including experiments of photoaffinity labeling, mass spectroscopy, and binding studies. My current research remains focused on Gram-negative bacteria, this time investigating their virulence and pathogenicity related to the presence of unexplored surface glycoprotein and bacterial glycans. (Read Gloria's article DOI: 10.1021/acschembio.7b00822.)

NOELIA BERNARDO-GARCÍA

Image courtesy of Elsa Franco-Echevarría.

Education: 2009, B.S. Biotechnology, University of León, Spain; 2015, Ph.D. Biology, Complutense University of Madrid, Spain, Advisor: Prof. Juan A. Hermoso

Curent Position: Postdoctoral Fellow, CNRS-ENS Laboratory of Biology and Applied Pharmacology, France, Advisor: Prof. Jacqueline Cherfils

Nonscientific Interests: Illustration, art, and running

My research interests lie in unraveling the molecular mechanisms of virulence and pathogenesis. My Ph.D. Thesis focused on the structural biology of bacterial surface proteins involved in key functions, such as binding of the pathogen to host cellular receptors or remodeling of the peptidoglycan framework, which represent important mechanisms in the process of disease. I am very excited about publishing this work in *ACS Chemical Biology*, which reports structural insights into the transpeptidase mechanism of the PBP2x in *Streptococcus pneumoniae*, an enzyme critical in septal peptidoglycan synthesis during cell division. We have identified an allosteric site in the PASTA domains of PBP2x that would allow recognition of the nascent peptidoglycan strands triggering the transpeptidation process in division. The work provides a new facet in the role of PASTA domains and points that facilitation of catalysis by allostery is likely more common in bacteria (and in nature) than what the dearth of examples implies. (Read Noelia's aricle DOI: 10.1021/acschembio.7b00817.)

SHREYANS K. JAIN

Image courtesy of Khyati Mehta.

Education: Lachoo Memorial College of Science and Technology, India, B. Pharm, 2004; National Institute of Pharmaceutical Education and Research, India, M.S. (Pharm), 2007, in Natural Products; Indian Institute of Integrative Medicine-Council of Scientific and Industrial Research, India, Ph.D. Chemical Sciences, 2015

Current Position: Postdoctoral Fellow, Georgetown University, Departments of Oncology and Biochemistry, Waters Center of Innovation in Metabolomics, Washington, DC, USA, Advisor: Dr. Amrita K. Cheema

Nonscientific Interests: Cricket, reading history of religion and philosophy, chess, and walking

Natural products have been a valuable source of chemicals for drug discovery. My research focuses on drug discovery from natural sources with overall objectives to build a library of compounds for screening to identify natural leads. Experimental designs include extraction, enrichment, and purification using different chromatographic techniques, including HPLC, dereplication, and identification of metabolites by using LC-MS, MS-MS, and complete structural elucidation by detailed 2D NMR studies. Although we were able to find some natural preclinical lead molecules for further drug discovery using conventional biological screening, the current project focuses on screening using LC-MS to discover quorum-sensing inhibitors, using real-time identification and quantification of biomarkers with HRMS and MRM. A significant quantitative change in the production of biomarkers in *Pseudomonas aeruginosa* PAO1 was observed in the presence of capsaicin and 6-gingerol, correlating with antiquorum-sensing properties of molecules. This study demonstrates LC-MS as a tool for screening and discovering quorum-sensing inhibitors. (Read Jain's article DOI: 10.1021/acschembio.7b00875.)

MANOJ KUSHWAHA

Image courtesy of Nisha Sharma.

Education: B.Sc. in Biotechnology, 2008 (Dr. Hari Singh Gour University, Sagar (Madhya-Pradesh), India and M.Sc. in Biotechnology, 2011 (Dr. Hari Singh Gour University, Sagar (Madhya-Pradesh), India. Registered for Ph.D at Guru Nanak Dev University, Amritsar, Punjab, India

Current Position: Project Assistant and Ph.D. Scholar, CSIR-Indian Institute of Integrative Medicine (Jammu) and Department of Biotechnology, Guru Nanak Dev University, Amritsar (Punjab), Advisors: Dr. Ram. A. Vishwakarma and Dr. Sundeep Jaglan

Nonscientific Interests: Mountain tracking, gardening, listening to music, playing badminton and cricket, chess, and arts and crafts

My research focuses on LC-MS/MS based discovery of natural products from microbes. I have developed different LC-MS based methods for qualitative and quantitative analysis of natural and synthetic compounds, drug recovery studies in plasma samples, drug metabolite studies through MS-MS, chemical profiling of plant/microbial extracts, structure elucidation of compounds on the basis of mass fragmentation patterns, LC-MS

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based identification of stable isotope labeled chemical compounds, and others. I am also gaining experience in protein identification and protein characterization (biopharmaceuticals) techniques through high-resolution mass spectrometry and have become adept with the handling, operation, and troubleshooting of the mass spectrometry instrument. In our article, we have focused on LC-MS/MS identification of metabolites of *Pseudomonas aeruginosa* PAO1, time dependent production of signaling molecules (pyocyanin/rhamnolipids/N-acyl homoserine lactones), and LC-MS/MS based screening of quorum-sensing inhibitors. (Read Manoj's article DOI: 10.1021/acschembio.7b00875.)

HENGYU LU

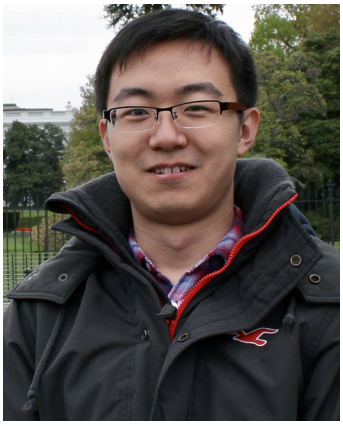

Image courtesy of Chennan Ding.

Education: The Hong Kong Polytechnic University, B.Sc. Applied Biology with Biotechnology, 2012; Baylor College of Medicine, Ph.D. Integrative Molecular and Biological Sciences, 2017, Advisor: Dr. Kenneth L. Scott

Current Position: Postdoctoral Scholar, Novartis Institutes for BioMedical Research (Cambridge, MA), Advisors: Dr. Huaixiang Hao and Dr. Giordano Caponigro

Nonscientific Interests: Cooking, coffee tasting, and movies

I'm interested in exploring combined therapeutic strategies in cancer, specifically for MAPK inhibitors to achieve durable pathway inhibition and better antitumor efficacy. My current research focuses on understanding the SHP2 biology in cancer, particularly its role in mediating feedback activation in RAS mutant cancers following treatment of MAPK inhibitors. In this article, we identified a second, distinct small molecule allosteric site on SHP2 and showed that simultaneous occupation of both allosteric sites could cooperatively enhance the MAPK pathway inhibition. Our work illustrates an example of dual allosteric targeted protein inhibition and enables our effort to further interrogate the functional role of SHP2 in cancer. (Read Hengyu's article DOI: 10.1021/acschembio.7b00980.)

HANNES LUDEWIG

Image courtesy of Hannes Ludewig.

Education: University of Bayreuth, Germany, B.Sc. Biochemistry, 2012; M.Sc. Biochemistry and Molecular Biology, 2014, Advisor: Prof. Dr. Wulf Blankenfeldt

Current Position: Ph.D. Student, University of St Andrews, UK, School of Chemistry, CRITICAT CDT (George and Stella Lee Scholarship), Advisors: Rebecca J. M. Goss and James H. Naismith

Nonscientific Interests: My cats and ultimate frisbee

The current focus of my Ph.D. project is to increase in-depth understanding of macrocyclase mechanisms to facilitate the development of biocatalytic tools enabling more efficient synthesis of cyclic peptides—valuable molecules for drug discovery. I am particularly interested in PCY1, a macrocyclase from plants displaying promising substrate promiscuity yet relying on large peptides substrates, challenging biotechnological applications. Structural and functional analysis of substrate enzyme complexes, employing X-ray crystallography, ITC, and LC/MS based assays, illuminated PCY1's mechanism, allowing the design of simpler substrates, enabling more efficient biosynthesis of cyclic peptides. (Read Hannes's article DOI: 10.1021/acschembio.8b00050.)

VANESSA PORKOLAB

Image courtesy of Jennifer Bailey.

Education: Grenoble-Alpes University (Grenoble, France), B.A. Biology and Chemistry, 2011, M.Sc. Bio-Organic Chemistry, 2013; Institute of Structural Biology (Grenoble, France), Ph.D. Biochemistry, 2016, Advisor: Prof. Franck Fieschi

Current Position: Postdoctoral Fellow, Brandeis University (USA), Chemistry Department

Nonscientific Interests: Twenty years of karate practice (Black Belt third Dan), karate and self-defense instructor for women. Martial arts, cooking, and traveling

My graduate research focused on the development of specific and multivalent antagonists against DC-SIGN, a C-type lectin receptor (CLR) that modulates the immune response. Some CLRs are hijacked by viral and bacterial carbohydrate-based pathogens. Thus, the design of ligands able to target specifically one CLR has potential value in therapeutic design. Selectively blocking DC-SIGN, being notably involved in HIV transinfection of T lymphocytes, without interfering with Langerin-mediated HIV clearance seems to be a challenging task due to their overlapping carbohydrate specificity. By studying both lectin-binding sites, however, a rational-differential approach has been exploited to design, synthesize, and tightly characterize a highly selective glycomimetic for DC-SIGN. Additionally to this work, we investigated multivalent scaffolds with different valences as well as ligand presentation in space to improve the affinity and thereby to compete with the HIV gp120 binding. Some of them show amazing affinities due to an avidity phenomenon of multivalent ligands for DC-SIGN. (Read Vanessa's article DOI: 10.1021/acschembio.7b00958.)

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NOREEN F. RIZVI

Image courtesy of Elliott B. Nickbarg.

Education: Cornell University, B.S. Chemical and Biomolecular Engineering, 2009; Northeastern University, Ph.D. Chemical Engineering, 2015

Current Position: Postdoctoral Fellow at Merck & Co., Inc. (since publication of this article, Noreen has accepted a position as a Senior Biochemist at Siemens Healthineers)

Nonscientific Interests: Traveling and exploring the many restaurants in New York City

My early research focused on enhancing the production of natural anticancer compounds through genetic engineering of plant cell cultures. Through my applications of RNA-interference, I became fascinated with the increasingly important biological role of RNA, which was once thought of as merely a messenger between DNA and protein. I coupled my interest in RNA and drug discovery by pursuing a postdoctoral fellowship at Merck & Co., Inc., where I investigated the treatment of human diseases by targeting RNA with small molecule drugs. In this publication, we apply a high-throughput affinity-selection mass spectrometry screening method, known as Automated Ligand Identification System (ALIS), to identify new ligands that bind to structured, regulatory RNAs. We identify novel small molecules that bind to our target RNA, and through biophysical and structural analysis, we demonstrate that conformational changes induced upon RNA−small molecule interactions govern phenotypic activity. (Read Noreen's article DOI: 10.1021/acschembio.7b01013.)

NISHA SHARMA

Image courtesy of Ankit Shakyawal.

Education: 2010, B.Sc. Biotechnology, University of Jammu; 2012, M.Sc. Biotechnology, Shri Mata Vaishno Devi University. Registered for Ph.D. at the Academy of Scientific and Innovative Research (AcSIR) under the guidance of Dr. Sundeep Jaglan

Current Position: Assistant Professor, Department of Biotechnology, G.G.M Science College, Jammu, India

Nonscientific Interests: Teaching, social work, gardening, listening to music, driving, and playing badminton

My current research interests are bioprospecting endophytic fungi for bioactive natural products. This involves identifying metabolites of microbial origin as well as isolating and screening for potential bioactive characteristics, such as being anticancer, antimicrobial, antibiofilm, and antioxidant, among others. For enhanced production of interested metabolites, media engineering is one of the strategies on which I am focusing. (Read Nisha's article DOI: 10.1021/acschembio.7b00875.)

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