### PLENARY LECTURE 1

## DEVELOPING AND APPLYING COMPUTATIONAL RESOURCES FOR BIOCHEMISTRY EDUCATION

PROF. PAUL A. CRAIG

Rochester Institute of Technology New York UNITED STATES OF AMERICA

Biochemistry is about structure and function, but it is also about data - lots of data - and this is where computers come in. From my time as a graduate student and post-doc, whenever I encountered data I thought, "I can work this up by hand, but I think a computer could do a better job," even though I knew very little about coding. Since that time, I have been working at the interface of biochemistry and computers, by attracting talented students and collaborating with colleagues with complementary skills. This has resulted in several projects I would like to present: the human visualization project, a simulation of 2D electrophoresis and tandem mass spectrometry, and two different programs that enable biochemists to search protein structures for enzyme active sites, ProMOL (promol.org) and Moltimate (moltimate.appspot.com). In addition to describing and demonstrating the websites and software we have developed, I will also discuss the human side of the project — how to find and work with the right students and colleagues for a project. This includes effective communication across disciplines, building and managing effective teams and the importance of serendipity throughout the process. I will conclude with a discussion of how the enzyme active site alignment tools formed the basis of the BASIL (Biochemistry Authentic Scientific Inquiry Lab) and changes in student and faculty behaviors and learning that have emerged from this project.



Paul Craig is a professor and head of the School of Chemistry & Materials Science at the Rochester Institute of Technology (RIT). He earned his B.S. in chemistry from Oral Roberts University in 1979 and his Ph.D. in biological chemistry with Eugene Dekker from The University of Michigan in 1985. Following a post-doctoral fellowship studying the biophysical chemistry of blood clotting (Henry Ford Hospital) and five years as an analytical biochemist at BioQuant, a technology transfer company associated with The University of Michigan, he joined the Department of Chemistry at RIT in 1993, with plans to "use computers to teach biochemistry." He has taught courses in biochemistry, analytical chemistry and bioinformatics. His students have developed computer simulations of protein separations (chromatography and electrophoresis - both ID and 2D) and software for molecular visualization and predicting protein function. He helped to found the BioMolBiz working group (https://qubeshub.org/ community/groups/biomolviz) which promotes molecular visualization literacy. He currently leads the BASIL consortium (Biochemistry Authentic Scientific Inquiry Lab; http://basiliuse.blogspot.com; https:// basilbiochem.github.io/basil/), a growing team of faculty members from more than ten campuses who are implementing a course-based undergraduate research experience (CURE) where students use in silico and in vitro techniques to predict and test protein function. He has been married to his wife, Elsa, since 1986, and they are very proud of their four children.

### **PLENARY LECTURE 2**

# FISH-HUNTING CONE SNAILS: HOW CORRELATING BEHAVIOR WITH VENOM PEPTIDES FACILITATES BIOMEDICAL APPLICATIONS.

### BALDOMERO M. OLIVERAI, SHRINIVASAN RAGHURAMANI, HELENA SAFAVI3

<sup>1</sup>University of Utah, Salt Lake City, UT

A number of bioactive peptides derived from cone snails (Conus) that live in tropical marine environments have become leads for non-opioid therapeutics for pain. One of these Conus peptides, originally discovered and characterized in our laboratories, is an approved drug (Prialt, generic name Ziconotide); it specifically targets a voltage-gated calcium channel, Cav2.2. Two other bioactive Conus peptides which are analgesic have reached human clinical trials: Contulakin G which targets the neurotensin receptor and Conantokin G which targets NMDA receptors that have an NR2B subunit. The fish-hunting lifestyle of some cone snail species was established by the ground-breaking work of Alan Kohn when he was doing his Ph.D. graduate research in Hawaii. It has become clear that there are over 100 species of cone snails that primarily prey on fish. The different lineages of fish-hunting cone snails have evolved a variety of divergent strategies to capture their prey. We will describe these alternative fish-hunting strategies, and show how the bioactive venom peptides evolved by a cone snail species correspond to the behavioral repertoire of that Conus. An overview of how the discovery and characterization of biomedically-significant peptides can be accelerated by knowing how the fish-hunting cone snail uses its venom peptides to capture fish will be presented for the different strategies for capturing prey evolved by the various lineages of piscivorous Conus. Some new potential applications of venom peptides from fish-hunting cone snail venoms to address the opioid crisis will be summarized.



Baldomero ("Toto") Olivera grew up in the Philippines; he received his B.S. degree in Chemistry from the University of the Philippines, his Ph.D. working on the Biophysical Chemistry of DNA at Caltech, followed by postdoctoral work in Biochemistry at Stanford. His early research contributions include the discovery and biochemical characterization of E. coli DNA ligase, a key enzyme of DNA replication and repair that is widely used in recombinant DNA technology. He is presently a Distinguished Professor of Biology at the University of Utah. Toto Olivera initiated the characterization of the venoms of the predatory cone snails. A large number of peptide neurotoxins ("conopeptides") are present in these venoms, and their characterization led Olivera's research group to a broad involvement with molecular neuroscience. Conus venom components are used to investigate the function of individual ion channels and receptors. The cone snail project has raised wide-ranging biological questions, from mechanisms of protein folding and post-translational modification, to gene organization and mechanisms of speciation. Several peptides discovered in Olivera's laboratory reached human clinical trials and one (Prialt) has been approved for the treatment of intractable pain. He is a member of the American Philosophical Society, the U.S. National Academy of Science, and the Institute of Medicine. He was given the Outstanding Alumni Award of Caltech, the Redi Award from the International Society for Toxinology and the Harvard Foundation Scientist Award of the Year 2007.

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### **PLENARY LECTURE 3**

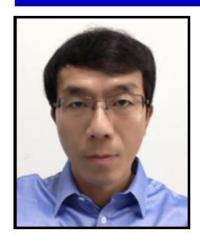
## HOW TO IGNITE STUDENTS' INTEREST IN BIOCHEMISTRY-LEARNING

PROF. RONGWU YANG

Nanjing University
PEOPLE'S REPUBLIC OF CHINA

Biochemistry is the most important subject in life sciences and also is very difficult for instructors to teach and for students to learn. As an instructor, you have to do your best to ignite students' interest in biochemistry learning. But how?

This presentation will offer you many means you can use or try to arouse your students' interest in learning biochemistry. For example, you can organize biochemistry song contest among students.



Dr. Rongwu Yang is currently Professor in Biochemistry and Molecular Biology, based in the School of Life Sciences at Nanjing University, in the People's Republic of China. He received his BS in Biology from Nanjing Normal University in 1986, MS in Biochemistry from Shanghai Institute of Biochemistry of Chinese Academy of Sciences in 1993 and PhD in Biochemistry and Molecular Biology from Nanjing University in 2006. His research field focused on signal transduction and molecular recognition. In 1993, Dr Yang began to perform biochemistry teaching and research at Nanjing University. His teaching performance has been widely recognized and highly praised on a nationwide scale, so he won many teaching awards. He is very popular with his students and was twice selected as the best loved teacher at Nanjing University, in 2015 and 2016. He has participated in many national and provincial projects involving research into biochemistry and molecular biology teaching, as well as the development of teaching material, such as Jiangsu province's higher education reform research project. He has published many teaching papers and textbooks such as Principles of Biochemistry, Biochemistry and Molecular Biology in Chinese. As an expert of Ministry of Education of China in middle school biology courses, Dr. Yang participated in validating new biology course standards and textbooks for junior middle school, as well as formulating new biology course standards for senior middle school.