

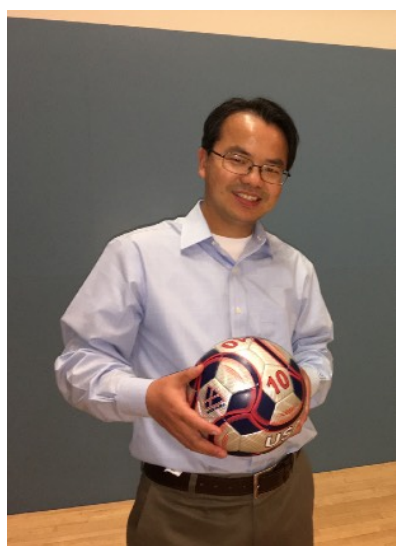
Meet Dr. Wu  
VP, Computational  
Drug Discovery

Partner Goals:  
Reaching Critical  
Milestones

T.G.I.F at  
Pharmaron

Supporting  
Future  
Scientists

Focus On:  
Compound  
Management System



## Meet Dr. Guosheng Wu

Do you remember the first email you sent? Dr. Guosheng Wu remembers it well. It was 1997 and it was to Professor George Schatz at Northwestern University. He credits that email as the start of his path to becoming a computational chemist. Fast forward almost 20 years, now Guosheng and the Pharmaron Computer-Aided Drug Design (CADD) and Structural Biology teams are driving drug discovery innovation with state-of-the-art tools that make that once-impressive email technology look basic.

As a student, Guosheng was fascinated by the structure of molecules and especially C60, and he admits he was drawn to its soccer ball shape. He went on to not only pursue his degree in computational chemistry, but travel over 6,000 miles to get his Ph.D. from Northwestern, where he was able to study with well-known theoretical and computational chemist, Professor Schatz.

In 2011, Guosheng took Pharmaron to new heights by becoming the first member of its CADD team, which has been steadily growing. Today, Guosheng and his colleagues are applying innovative tools to propel our partners' drug discovery efforts.

A recent client study from Genentech, published in the Journal of Medicinal Chemistry in February 2016 [2016, 59 (6), pp 2760–2779], showcases the positive impact CADD has on drug discovery. The Genentech and Pharmaron teams were able to quickly move the project to a late-stage by working closely with the CADD team at Pharmaron.

What's the key to the CADD team's success?

"My team's in-depth technology experience and scientific insight are what set us apart. Through computational design studies with numerous protein targets, our team has built a knowledge base in positive and negative interactions between a drug target and a ligand, as well as drug-like properties for ligands. With this we can pick strong designs and improve the ideas from the computer programs. I have essentially transformed myself and my team into computational medicinal chemists."

### About Dr. Wu

Dr. Guosheng Wu joined Pharmaron in 2011 as Executive Director and is now Vice President of Computational Drug Discovery. Prior to Pharmaron, he worked at Eli Lilly and Vitae Pharmaceuticals. He received his Ph.D. at Northwestern University. He has over 30 patent applications and peer-reviewed publications. In his free time, he enjoys traveling and learning the history and culture. As for soccer, he's not a player, but he still appreciates its C60 shape similarity.

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## 2 Reaching Critical Milestones

There is no better feeling than knowing our research makes a difference, and that's especially true when we help our collaborators and partners reach critical milestones along the drug R&D process, such as entering First-in-Human (FIH) studies.

Merck Sharp & Dohme (MSD) Research Laboratories and Genentech are two examples of partners using Pharmaron's high quality services. In addition, we are pleased to hold numerous patent applications and publications with our partners. Currently Pharmaron and MSD Research Laboratories have 38 patent applications and publications. Pharmaron and Genentech have 41 patent applications and publications.

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## 4 Supporting Future Scientists

Since 2011, Pharmaron has established a post-doctoral scholarship program, with the mission to support outstanding Ph.D. students to gain world-class scientific research experience and training and to encourage aspiring students to pursue further education in organic chemistry.

This year two Pharmaron scholarship recipients from Shanghai Institute of Organic Chemistry, Dr. Bo Pang and Dr. Jun Zhu, are pursuing their post-docs from Joint BioEnergy Institute of Lawrence Berkeley National Laboratory and University of Chicago, respectively. Both of them came to Pharmaron to discuss their Ph.D. work with chemists in a recent Friday Seminar Series presentation before they went abroad.

Dr. Pang presented "Biosynthesis on Assembly Line – the Organic Synthesis Pipelining in Nature." Dr. Zhu presented "Development of Novel Cascade Cyclization Reactions Based on Indole Derivatives." Dr. Boliang Lou, Chairman and CEO said, "We are proud to continually support the next generation of scientists, who are the key to our future."

## 5 Focus On: Compound Management System

Critical to novel drug discovery and development is *in vitro* bio-testing, which often involves a large number of samples in a plate format, along with data to be prepared, processed, stored and retrieved. Precision, accuracy, reproducibility and efficiency are key criteria for the success of the *in vitro* assays. Pharmaron has developed Compound Management System, a tailor-made system that includes strong IP protection to meet these criteria.

The system is composed of a high throughput liquid/plates handling platform and a secured sample storage platform, complemented by sophisticated data management and processing software, such as Mosaic and ActivityBase. A dedicated and well-trained team of scientists, together with a vigorous QC process imbedded throughout the entire system, ensures that each step supporting the assay needs of *in vitro* biology, *in vitro* ADME and *ex vivo* pharmacology is of high quality. The Compound Management System has contributed to the success of a significant number of assays run with outstanding precision, accuracy and reproducibility, for panel/counter and project-based screenings.

## 3 T.G.I.F.

"Thank Goodness it's Friday" is a sentiment many Pharmaron scientists have, but not for the reasons you may think. The Friday Seminar Series at Pharmaron is a weekly opportunity for Pharmaron scientists to learn from not only fellow colleagues – but industry and academic leaders as well.

From hearing a colleague discussing a recent success – to hearing an academic leader or industry leader discussing recent advances in life sciences and challenges faced in the current marketplace, it's a chance for the team to see how Pharmaron is helping our partners meet their drug discovery and development objectives – as well as ways to drive innovation with their collaboration projects.

*Recent Presenters:*

- **Prof. Yi Rao**, School of Life Sciences, Peking University, China, "Molecular Genetic Analysis of Sleep"
- **Prof. David Schubert**, Salk Institute for Biological Studies, US, "Drug Discovery for Neurodegenerative Diseases"
- **Prof. Jean J. Zhao**, Dana-Farber Cancer Institute, Harvard Medical School, US, "Targeting Therapeutic Resistance in Cancer: From Mouse Models to Human Therapy"
- **Dr. Joseph L. Duffy**, MSD Research Laboratories, US, "The Discovery of State-dependent, Orally Bioavailable Cav2.2 Inhibitors for the Treatment of Chronic Pain"

