USC develops software to facilitate large-scale biological inquiry

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ProteoWizard Toolkit first able to interpret multi-platform mass spectrometry data

The world's leading mass spectrometer manufacturers have agreed to license technology that enabled University of Southern California (USC) researchers to develop software that, for the first time, allows scientists to easily use and share research data collected across proprietary platforms.

The ProteoWizard Toolkit, a cross-platform set of libraries and applications designed to facilitate the sharing of raw data and its analysis, is expected to bolster large-scale biological research and help improve the understanding of complex diseases like cancer.

"Think of it like a Rosetta Stone—it translates multiple languages, but unlike the original, ProteoWizard is easy to use, widely available and easily expanded upon," said Parag Mallick, Ph.D., ProteoWizard's lead developer and director of clinical proteomics at the Center for Applied Molecular Medicine in the Keck School of Medicine of USC.

Proteomics is the branch of biochemistry that studies the structure and function of proteins, thousands at a time, a cumbersome endeavor due to the volume of data involved. Innovation within the field has been hampered by the multiple file formats used to process and store such data, making it nearly impossible to compare, share and exchange information obtained on different platforms or by different labs. Historically, researchers have had to spend from months to years implementing a vast array of standard computations before innovative algorithms could be developed, another roadblock for those hoping to enter the field of proteomics.

"We asked ourselves what needed to happen to spur innovation in proteomics. We decided that there needed to be a standardized set of software that made it easy to enter the field." Mallick said.

It was 2007 when the USC team began collaborating with other laboratories to kickstart the effort. The short-term goal was to create a stable, open-source system that was easy to use and easy to grow. The long-term goal? To be the best-of-breed data analysis tool in the world.

With help from the USC Stevens Center for Innovation, Mallick's team created the ProteoWizard Software Foundation, which was critical to secure licensing agreements with all the major mass spectrometer manufacturers: AB SCIEX, Agilent Technologies, Bruker Daltonik GmbH, Thermo Fisher Scientific and Waters Corp. The agreements allow users of the free software to import mass spectrometry data

regardless of format and to easily manipulate it.

Mallick and his team also have launched ProteoWizard Projects, which allows developers to build more specific applications on top of the core software.

"Mass spectrometry is a key part of biomedical inquiry around the globe," said David Agus, M.D., co-creator of the software, director of the Center for Applied Molecular Medicine and professor of medicine and engineering at USC. "It tells us the composition and quantity of the molecular components that make up biological material, which doesn't sound like much. But, for us, mass spectrometry helps us understand cancer. It helps us understand why tumors respond to some drugs and not others and helps us predict how a particular patient will respond to a drug. The development of ProteoWizard for the first time allows biological scientists around the world to work together as a team."

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