Scientists design new metabolic technology to open scientific data for everyone

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Patients want to see their medical information. Researchers want to share their data.

Now, scientists at Scripps Research have released a new technology designed to make these measurements easier to perform and more accessible to practitioners, scientists and the general public.

"This is really about data sharing and accelerating the process of discovery," says Gary Siuzdak, Ph.D., professor at Scripps Research and co-corresponding author of the new XCMS/METLIN open data analysis platform, published recently in *Nature Methods*.

XCMS-MRM and METLIN-MRM represent a cloud-based analysis platform that allows scientists to quantify molecules from biological samples and make their results publicly available.

"When we say 'publicly available,' we mean it. Anyone with a computer would have access," says Siuzdak.

Directed by Siuzdak, the Center for Metabolomics and Mass Spectrometry at Scripps Research specializes in using a technique called mass spectrometry to identify and quantify small molecules, whether they are drugs or naturally occurring metabolites. Metabolites are critical as they interact with every level of a person's physiology: the genome, transcriptome and the proteome. One could say metabolites are master manipulators of physiology and reflect an individual's health signature.

Tens of thousands of labs around the world generate data using mass spectrometry, so the platform could be useful outside medicine as well, say study first authors Xavier Domingo-Almenara, Ph.D., and J. Rafael Montenegro-Burke, Ph.D., of Scripps Research. Any field using mass spectrometry could benefit from these new resources, such as environmental sciences, pharmaceuticals, forensics, food control and sports medicine, they add.

Siuzdak and his colleagues have long aimed to keep their research tools

free and open to the public. Paul Benton, Ph.D., bioinformatics analyst at Scripps Research and co-corresponding author of the study, explains that hosting their platform on the cloud allows anyone, from collaborators to patients, to check the validity of the mass spectrometry results. "In an age where scientific results are being constantly questioned, open data has become an essential part the discovery process," Benton says.

The idea of open data sharing has caught on in recent years. Since its launch in 2004, the XCMS/METLIN platform has grown to over 25,000 users, and the molecules in its data repository have leapt from 14,000 to 150,000 in just the last year, partly thanks to a collaboration with Calibr, a division of Scripps Research.

The new resources take advantage of breakthroughs that let scientists speed up research—and increase precision—by identifying the key fragments of a molecule that set it apart.

"There's nothing else even close to this," Siuzdak says.

The study, "XCMS-MRM and METLIN-MRM: a cloud library and public resource for targeted analysis of small molecules," included additional authors from the University of Lausanne; Lausanne University Hospital, Geneva University Hospitals; Umeå University and Imperial College London.

More information: Xavier Domingo-Almenara et al, XCMS-MRM and METLIN-MRM: a cloud library and public resource for targeted analysis of small molecules, *Nature Methods* (2018). DOI: 10.1038/s41592-018-0110-3

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