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Real Simple Metabolomics

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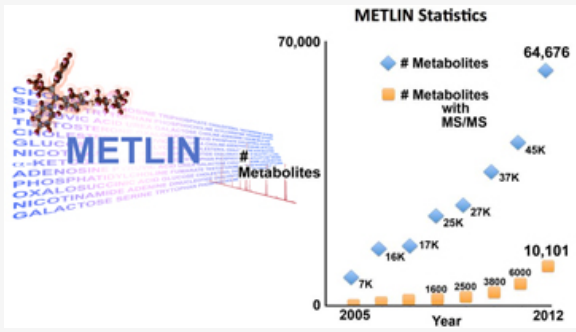
Researchers have expanded and improved a data library to simplify the process of metabolite identification, cutting the time from days to minutes.

In the early 2000s, Gary Siuzdak, a researcher at the Scripps Research Institute in La Jolla, CA, needed a way to identify unknown metabolites—small molecules produced during metabolism—in plasma. Using mass spectrometry (MS), a tool that measures the molecular weight of a compound, Siuzdak recorded the mass of a molecule in his sample but couldn't find reference data to identify it.

"I was trying to identify some of the unknowns that we observed, but unfortunately no one had a comprehensive list of biologically relevant molecules," said Siuzdak. Instead of giving up, however, Siuzdak decided to simply create the tool he needed. In short order, METLIN was born. "It was largely self serving," he said with a laugh, "but it turned out to help others with their research as well."



In the September issue of Nature Biotechnology, Siuzdak and colleagues describe the recent expansion and improvement of the METLIN online database for metabolomics. Source: Gary Siuzdak, Gary Patti

Free Virtual Symposium from BioTechiques - Oct 3, 2012

Gary Siuzdak from the Scripps Research Institute in La Jolla, CA will speak and answer your questions about his metabolomics research at our free virtual symposium on Oct 3.

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METLIN, a freely available online database of metabolites, premiered in 2004 with 7000 metabolites. Today, it includes a whopping 64,727, as well as numerous tools for identifying and analyzing the molecules. In the September issue of *Nature Biotechnology*, Siuzdak and colleagues describe the recent expansion and improvement of the database.

Prior to METLIN, as well as other metabolite databases such as the Human Metabolom eDatabase and Mass Bank, there was little information about metabolites online, leaving researchers to search through limited lists or textbooks. METLIN changed all that. "It's an enormous resource that saves time, money, and makes the whole process of metabolomics much more efficient," said METLIN co-developer Gary Patti, Siuzdak's former postdoc and now a professor at Washington University in St. Louis, MO.

METLIN distinguishes itself from other metabolite databases because it includes valuable high-resolution tandem MS (MS/MS) data—information about how a molecule breaks apart when collides with atoms or other molecules (e.g. argon or nitrogen. MS/MS data allows researchers to decipher between multiple molecules with the same molecular weight and “adds a much higher level of confidence” in metabolite identification, said Siuzdak.

For example, Patti used the MS/MS data in METLIN earlier this year to identify a novel metabolite involved in chronic pain (2), which has since proven to be a fruitful drug target. “We never would have gotten there if we had based it just on mass,” said Patti. METLIN includes MS/MS data for 10,638 metabolites, making it the largest MS/MS dataset in the world.

The database also incorporates software called XCMS, also developed in Siuzdak’s lab, that processes MS data prior to metabolite indentification. XCMS and METLIN together are being used to reduce the number of steps it takes to identify a metabolite from 6 to 2, cutting down metabolite identification time from days to minutes.

Siuzdak and Patti expect the database to continue to grow and are adding information from different types of instruments, such as nuclear magnetic resonance (NMR) data. They also want to add as many different metabolites as possible across a wide range of plants and animals. Recently, for example, ChromaDex, a botanical material manufacturer, contributed a wealth of plant metabolite information.

“In the early 2000s, we thought we knew just about everything about metabolism, but now the whole landscape is changing quite dramatically,” said Siuzdak.

Siuzdak will describe his latest metabolomics research using mass spectrometry and METLIN on Wednesday, October 3, 2012 at the *BioTechniques Virtual Symposium on The Cell Landscape: From Genotype to Phenotype*. Free registration here.

References

1. Tautenhahn, R., et al. 2012. An accelerated workflow for untargeted metabolomics using the METLIN database. Nat Biotech 30(9):826-8.

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Keywords: metabolomics