

Ezine

Metabolomics for all: A new web-based platform for analysing LC-MS data

Published: Jun 4, 2012

Author: Jon Evans

Channels: Laboratory Informatics

Lack of expertise

A new easy-to-use, web-based platform for processing and analyzing liquid chromatography-mass spectrometry (LC-MS) data will open up metabolomics to scientists with little knowledge of the intricacies of bioinformatics, say the US developers. In one simple automated process, this platform detects peaks, aligns retention times between samples, determines metabolites that are present at different concentrations in different samples, assigns possible identities to those metabolites, and performs multivariate statistical analysis.

Termed XCMS Online, this new platform is based on the earlier XCMS, which was developed by Gary Siuzdak and his colleagues at the Scripps Research Institute at La Jolla, California, in the mid-2000s. XCMS is open-source software for processing and analyzing LC-MS data produced by metabolomic studies, and has already been used to investigate the metabolites involved in biological processes such as cancer, chronic pain, fruit development, and stem cell differentiation (see *Stem cells prefer unsaturated*). But like other software packages for processing LC-MS data, XCMS requires the user to have a certain amount of bioinformatics and programming expertise, hindering its adoption by many scientists.

Sit back and wait

With the development of XCMS Online, Siuzdak and his team have removed the requirement for any specialist knowledge, allowing it to be used by any scientist conducting a metabolomic study with LC-MS. As it is entirely web-based, scientists don't even need to download any software onto their computer.

The scientist's involvement extends to just uploading the raw LC-MS data to XCMS Online, which can be done by simply dragging and dropping the data files to an upload area, and selecting appropriate experimental parameters, such as signal-noise threshold and mass tolerance for identification.

Even this step is not always necessary, as the parameters for certain commonly used instrument set-ups, such as HPLC-time of flight MS, are pre-set. The uploading and analyzing steps can each take from minutes to hours depending on the size of the data, with the platform accepting file formats utilized by all the major manufactures of mass spectrometers. When the analysis is finished, the scientist is notified by email.

Circles and plots

Similar to the original XCMS, XCMS Online uses various different algorithms to detect individual peaks, align retention times, detect metabolites that are under- or over-regulated between different samples, and identify metabolites by comparing the experimental data with an MS database called METLIN. It presents the data in an easily understandable, graphical format, showing the total ion chromatogram for each of the samples both before and after retention time correction, as well as the retention time correction curves.

The platform also shows plots of metabolites detected at different concentrations in different samples, with up-regulated metabolites displayed as green circles at the top of the plot and down-regulated metabolites displayed as red circles at the bottom of the plot. The size of the circles reflect the degree of change in concentration between the two samples, while circles with a black outline have been provisionally identified in METLIN. Hovering the cursor over these circles brings up the proposed identity, as well as other experimental features about the metabolite.

Finally, there are plots of the data after analysis by two multivariate statistical techniques – multidimensional scaling and principal component analysis – revealing underlying relationships and groupings within the data. Scientists can also easily drill down into the data, by bringing up a list displaying all the experimental information for each detected metabolite, including an ion chromatogram, the mass-to-charge ratio and the putative METLIN identification.

With XCMS Online freely available at <https://xcmsonline.scripps.edu>, there's now no excuse not to start that metabolomics study.



Related Links

Analytical Chemistry (Article in Press): "XCMS Online: A web-based platform to process untargeted metabolomic data"

Article by Jon Evans