Take a Pass on the 3pm Samples

Innovation in laboratory informatics technology is eliminating the battle for scientists with late afternoon sample analysis requests.

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Gone are the days when chemists would wait patiently for paper reports on their particular sample results to be sent to them. The introduction of informatics technology brought with it results that can be delivered by email and uploaded through a central system or stored in the cloud, so that they could be presented quickly and allow for timely decision making. Advances in laboratory informatics technology have changed, and continue to change, the way in which laboratories gather and interpret actionable information. Today's laboratories are looking for informatics technology that are easy-to-use, speed up their work, and deliver accurate results.

The use of modern informatics technology means that scientists no longer have to battle with sample analysis requests that come in at 3p.m., working hours of overtime to pull the information together. In the past, sample research information would take a substantial amount of time to analyse and, with respect to pharma, therefore risk slowing

down the drug pipeline. Today, scientists are able to access the information that they are seeking within minutes.

What are Labs Looking for?

Laboratories want a data system that is easy to use, that speeds up their workflow and guarantees confidence in its results. Designed from the ground up to make mass spec analysis easier from tuning to a final report, Agilent's MassHunter Software delivers just that.

One of the innovations Agilent offers in its software suite is the MassHunterWalkup software . This program makes it easy for non-MS experts to use a mass spectrometry to get the answers they need to make decisions. Many core labs are currently setting up Walkup systems so that they are able to share results directly with the user a few hours after a sample has been inserted into the auto sampler. This is a real success for many labs as it removes the burden of setting up and organising in-house analysis. This provides an "ATM" type of function for non-software users, removing the long wait for analytical results to come through.

Many companies work under a core lab model which means that they have dedicated laboratories within their facility and that they hire MS experts who are responsible for conducting the analysis. Within this model there is the ongoing risk that analysis will back up and cause chemists to have to wait a long time to get their results — subsequently delaying further decisions down the line.

Currently we are seeing many core laboratories setting up these types of high-throughput informatics systems such as MassHunterWalkup so that a chemist with a newly created sample can walk in, put it into an autosampler, fill in a few fields with information and hit 'Go'. Within a few hours they will receive an email with their analytical results.

Pharmaceutical laboratories want answers fast, but they also want a simple process through which to get them. Suppose you are a scientist synthesising a new compound, then you need to confirm an answer before making a decision on your next steps. If it takes two to three weeks to get the result it is difficult to move forward. Often this means you will either work on something else or assume that the work you are conducting is going well, and continue to work on it without knowing the outcome of the results. When this happens, and the results differ to what you had predicted, all the time spent and invested in the sample has been wasted.

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In addition to the MassHunterWalkup software offering, Agilent also has a personalised quantitative analysis called "Quant-My-Way". The software is a set of tools designed to assist the user in exposing only the capabilities of interest so that you can create your own tailored, streamlined version of MassHunter Quantitative Analysis for each specific assay. This allows the customer to modify the information to see exactly what they want to see. Using this tailored model to create result reports that contain specific information of interest reduces the time required to find the answers you need.

As well as wanting answers faster, pharmaceutical laboratories need confidence in the reliability of their results. In protein therapeutics, there are several ways to characterise the attributes of a new biomolecule. A 'bottom up' approach will take the protein, chop up it up with specific enzymes and then analyse each peptide. You can then put the information together in order to confirm the sequence and determine the identity and location of Post Translational Modifications (PTMs). MassHunter BioConfirm is software for the analysis of biopharmaceutical samples. Agilent has just introduced a new algorithm for this peptide mapping workflow. Using the MS/MS data from an LC/Q-TOF, which is much more specific and information-rich than MS-only data, it is able to rapidly identify peptide sequences and PTMs. This allows the calculation of the overall coverage of the protein as well as the locations of the PTMs on the sequence.

Visual Assets Provide Answers

However, it is not enough to just get lists and lists of new data – humans are visual animals which need excellent visualisations to rapidly assess new information and make decisions. The peptide mapping results are displayed on a new Sequence Coverage Map, which clearly outlines which parts of the sequence are confirmed, as well as whether the evidence is from MS/MS or MS-only data. It is possible to load multiple data files into the Sequence Coverage Map to get a cumulative coverage, e.g. from a multiple enzyme digest or Agilent's Iterative MS/MS mode that digs deeper into the sample with each subsequent MS/MS run.

Agilent's MassHunter VistaFlux software, which is used in pharma research through to drug discovery, is another example of an innovation in lab informatics that is changing the way scientists work. VistaFlux helps scientists map metabolic pathways and then visualise them in different ways. It can be used to test hypotheses on the Mechanism of Action (MOA) of new ▶

drugs and has recently been applied in the development of a new diabetes treatment by a major pharmaceutical company. This software tells the user over time what is occurring on the pathways through insights from algorithms, which transform into visual results that are easily discerned. These visualisations of the results create an efficient, time-saving working environment for all users.

Maximising the Opportunities in Laboratory Informatics

Pharmaceutical companies need to be able to ensure the safety of its products. This requires rigour for every aspect of their product's development and use– from drug development through to the packaging used to contain the drug itself.

To ensure this, biopharma companies are transitioning to the production of protein therapeutics with Single Use Technologies (SUT) such as plastic disposable bioreactors, membrane absorbers, media bags, bioprocess containers, disposable mixers, and samplers. However, it is very important that no unwanted compounds leach out of the plastics that might be delivered inadvertently to patients. Similarly, the packaging materials, containers and recipients might also contaminate a small molecule pharmaceutical product.

And how does informatics technology play into this? Agilent recently launched an MS/MS library (the Extractables & Leachables PCDL) that helps pharmaceutical companies determine if any E&L compounds are present in the products they are supplying to patients as a result of the materials they are produced and packaged in. The ability to recognise this contamination gives these companies the opportunity to prevent them. The library is used with other parts of the MassHunter suite for fast and accurate results.

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AUTHOR BIO

Steve has significant experience in chemical analysis, chemometrics and bioinformatics. Prior to his current role, Steve worked in software R&D and support. Today, he manages the marketing of Agilent's MassHunter qualitative software. This portfolio embraces customers' needs in a wide variety of markets including pharmaceutical, biopharmaceutical, and chemical analysis.