

IMPROVING R&D EFFICIENCY

*IN COMPOUND SYNTHESIS,
CONFIRMATION AND
PURIFICATION*



Researchers in the medicinal chemistry field need to process a large number of samples within a limited amount of time.

They must analyze a wide range of compounds to identify and develop promising candidates for drug discovery. Workflow efficiency and accuracy can both be greatly improved with the right software in place.

That's why Shimadzu developed the Open Solution data analysis software to make drug confirmation fast, easy and effective. When combined with Shimadzu's industry-leading liquid chromatography mass spectrometry (LCMS) and high-performance liquid chromatography (HPLC) instruments,

Open Solution provides a simple operational workflow for more efficient compound confirmation.

Walk-up software for any experience level



Up until now, if you wanted to analyze samples, you would have to submit the samples to an analytical chemist and then wait — often for days — to get the results you needed. But now all that's changing.

Thanks to easy walk-up software solutions, you don't have to be an expert in HPLC or LCMS to run samples.

Walk-up software is instrument management software that enables multiple users to easily submit samples to an analytical workflow. Users of all experience levels can “walk up” and use the software with no instrument or software training required. They can quickly get the results they need without compromising accuracy or sensitivity.

A man in a white lab coat and glasses is seated at a desk, looking at a computer monitor. His hands are on a keyboard. The background is a laboratory with other people and equipment, all overlaid with a teal tint.

For medicinal chemists running large data sets, ***Open Solution software can make a big difference in improving workflow efficiency.***

The software provides a simplified interface, eliminating all the clicks and guiding you through the entire process. All you need to do is enter the sample information, and the system will start up, check the status and run the samples automatically. The software will even direct the instrument to clean itself and shut down at the end of the day. If anything goes wrong during the day, the software will send a notification to designated personnel to initiate any required maintenance or service.

Sends an email notification when analysis is complete



Open Solution sends an email notification once analysis is complete, so you don't have to wait to view the results. The email contains a hyperlink to the stored results. Users can simply click on this link to view the results in an internet browser.

This instant access helps enhance the efficiency of analysis. Results can be confirmed quickly without having to make time-consuming trips to the laboratory. You also have the option to print or export the report as a PDF file. Additionally, completed samples in the queue can be analyzed while continuing to acquire data.





Easily share data with other departments



Open Solution makes it easy to share analytical data with other departments by creating an open access environment. With open access, there's no need to install special software on every computer in your facility.

Chemists can view results or print reports using their web browser, which saves significant time, money and hassle. You don't have to worry about purchasing separate licenses for each computer, and you spend less time installing and maintaining software packages.

Simplify and speed up compound verification

Med chemists not only have to process a large number of samples. They also spend a considerable amount of time verifying analytical results using LCMS. When verifying analytical results, chemists need to review and compare data from multiple experiments to confirm the purity and identity of each compound. With traditional software this involves opening each file individually and switching between multiple windows and views. ***This process can become very time-consuming as the volume of data and the number of samples increase.***

It can also be difficult to correlate the data with the vial that contained the measured sample. For example, you may start the analysis with 10 sample vials, and then add more vials to the queue before the initial series of analyses is complete. As you add more vials, it becomes increasingly difficult to identify a particular vial using just the file name. ***It would be much more efficient if you could check the results and view the vial positions in the sample rack on the same screen.***

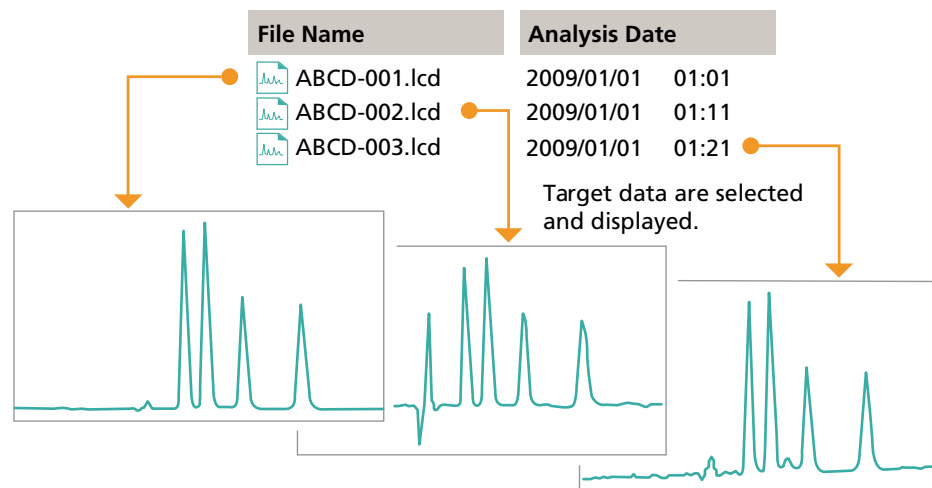


Fig. 1 Typical Method of Selecting and Displaying Data

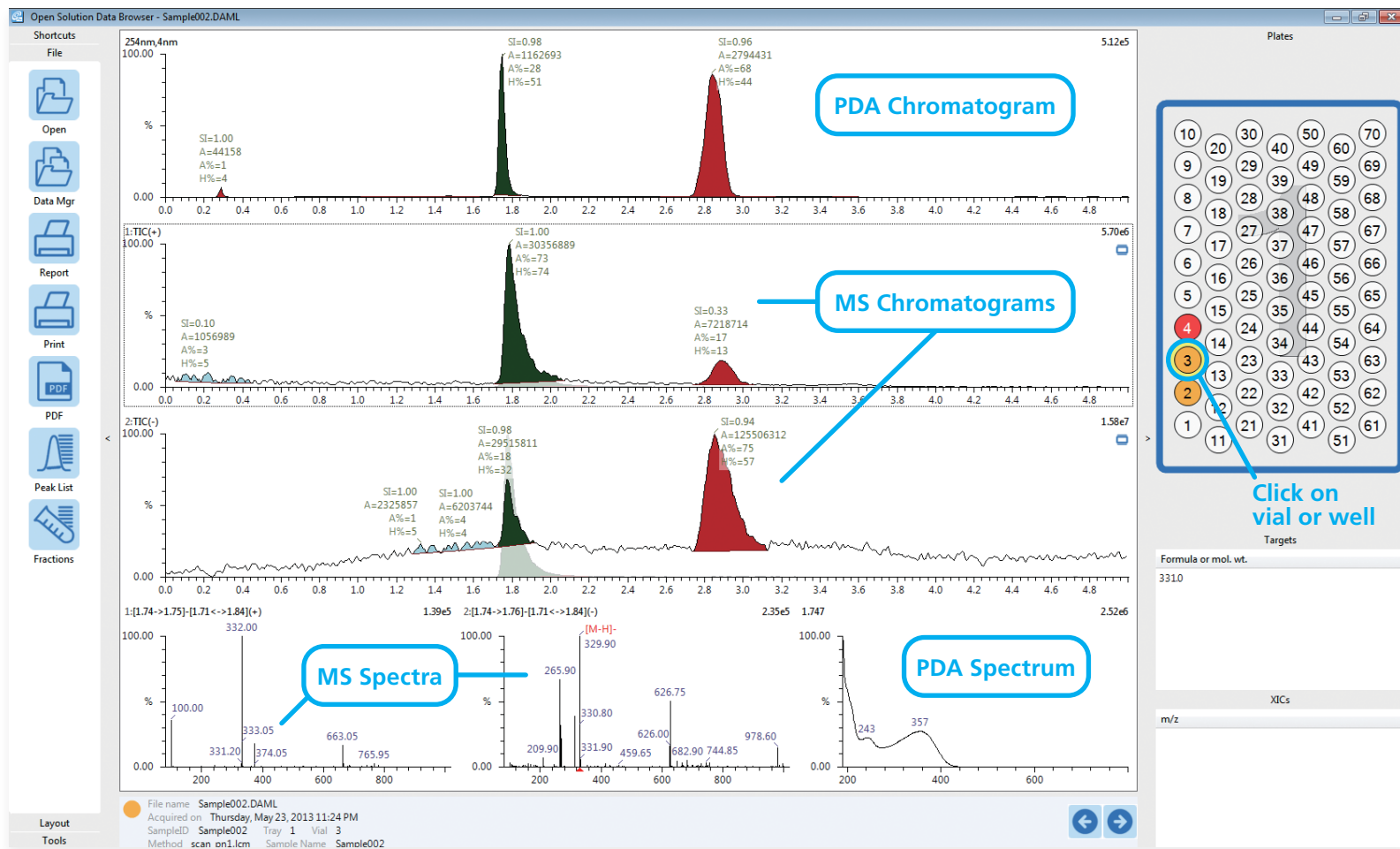


Open Solution shows a visual representation of vials



The software shows a visual representation of the vials in the autosampler tray. When you click on the image of the vial, the results (chromatograms, spectra, peak table) are displayed. If the target compound is detected, there will be a green checkmark next to the corresponding mass in the target MS table. ***This feature is very useful when you need to confirm the results of multi-sample analysis using microplates.*** Results from PDA and MS can be viewed in a single screen, and toggling between samples is as simple as clicking on the desired vial position.

Unlock the power of one-click data review.





Drug synthesis plays an integral role in drug development, but it can be a long, complex process. Shimadzu's Open Solution data analysis software ***helps you reclaim more hours in the day by streamlining and automating your workflow.***



To learn more about how you can improve productivity in your lab, visit ***www.SolutionsForPharma.com***

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7102 Riverwood Drive, Columbia, MD 21046, USA
Phone: 800.477.1227 / 410.381.1227
www.ssi.shimadzu.com