

Opening LCMS to Research: PsiPort Browser Software

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1. From Login to Report Generation, Making Research Easier and Faster

In the development of new pharmaceutical and chemical products, large numbers of novel compounds are synthesized every day. Researchers in such departments often require software that is easy to use and allows quick output of their LCMS results. When analytical instruments are shared among multiple users in a walk-up or walk-away environment, it is important to have software that can be operated by different operators with differing levels of proficiency. In such departments the value of easy-to-use software becomes as important as the instrument itself.

The concept that describes this best is “open-access analysis.” The requirements of open-access analysis can be summed up by the words “easier and faster”. PsiPort Browser is the software that satisfies these requirements, enabling true high-throughput operation to support high-throughput synthesis chemistry.

2. PsiPort Browser – Web-Based Browser Access

PsiPort Browser software enables operation of the LCMS-2010EV liquid chromatograph mass spectrometer directly. Using PsiPort Browser, method and report files are specified, and all operations from login to report output can be conducted as simply as filling in a sample queue in a spreadsheet.

One of the greatest features of the PsiPort Browser is its ease of operation.

PsiPort Browser is a web-based software platform that is used in conjunction with Microsoft Internet Explorer (web browser), so installation of specific application software is not required. Moreover, since operations

can be conducted via the web browser, as long as an in-house LAN or other internet access is in place, researchers can easily view the operating status of the LCMS, browse previously acquired data, and output reports at any time and from any location with internet or intranet access.

Furthermore, since the web browser is used for all data evaluation operations, the LCMS software does not need to be installed on any local PCs, thereby achieving a convenient LCMS environment with little capital investment.

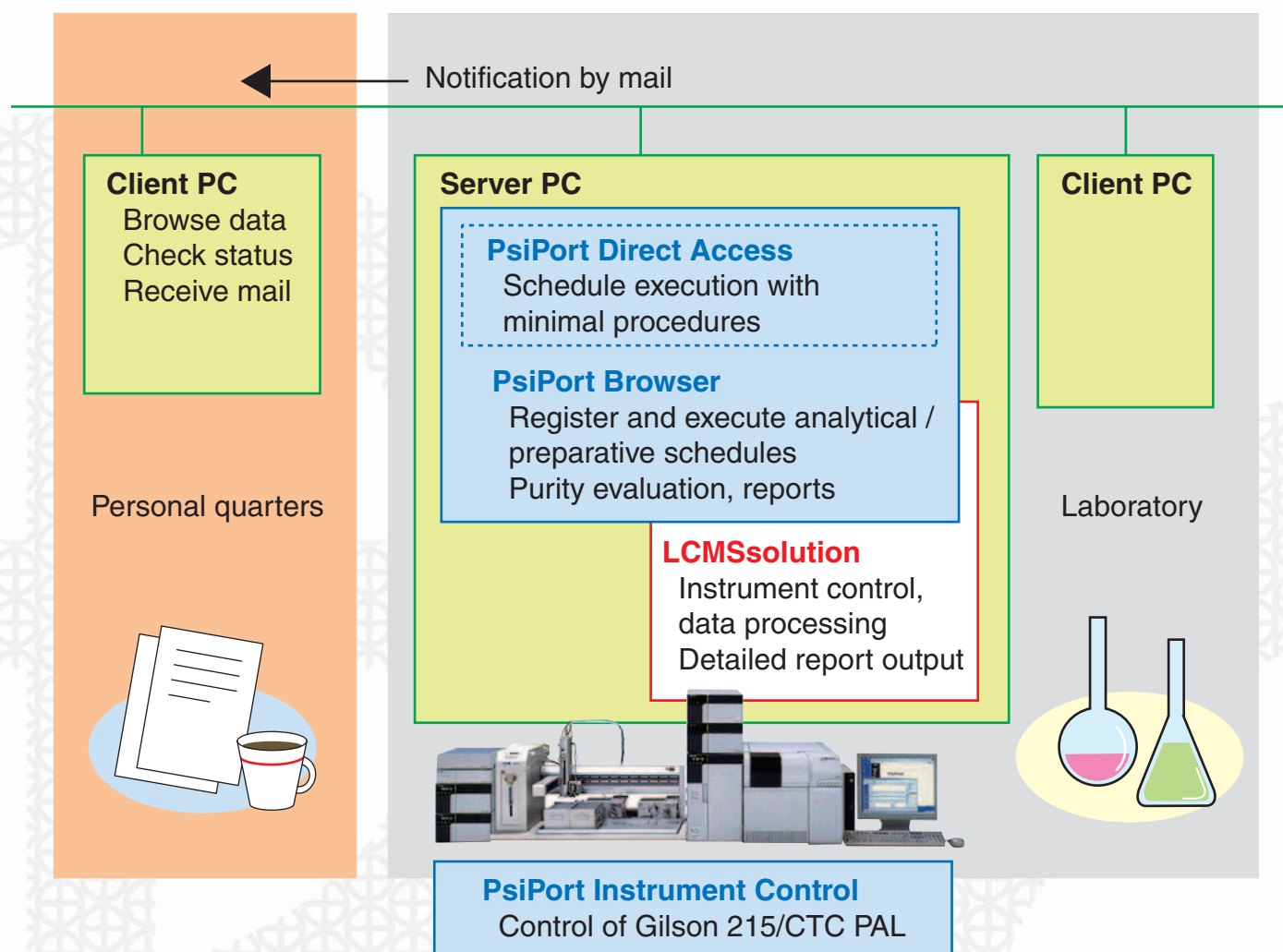


Fig. 1 PsiPort Browser Open-Access Operating Environment

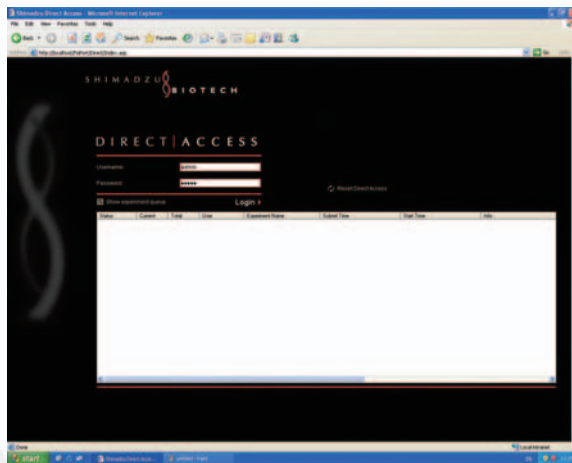
3. PsiPort Direct Access – Easier Sample Registration

To have even one less mouse-click –
For many researchers, the complexity of PC operations hinders the efficiency of research work. PsiPort Direct Access satisfies the demand for easy PC operation by minimizing the number of inputs necessary to run a sample.
Just a few screen-switching operations, and the user glides through login to the start of analysis.

The actual flow...
(Step 1) Log into PsiPort Direct Access.
(Step 2) Enter the number of samples to be analyzed.
(Step 3) Select the method file.
(Step 4) Verify the sample vial positions.
(Step 5) Click the Finish button.
These 5 steps are it!

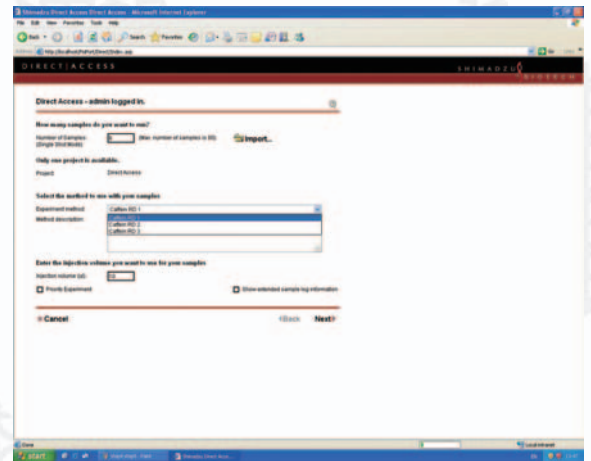
Everything else is performed by the LCMS-2010EV Mass Spectrometer. By the time you get back to your quarters, the analysis might even be complete and the results already on your computer.

(Step 1)
Login



(Step 2)
Input number of samples

(Step 3)
Select method file



(Step 4)
Set vial positions

(Step 5)
Click Finish

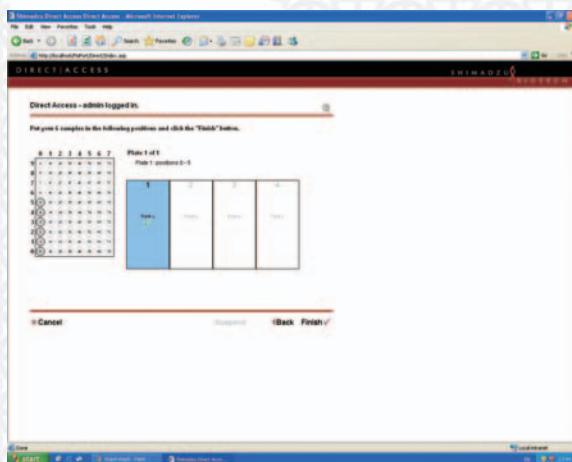


Fig. 2 PsiPort Direct Access Sample Registration Flow

4. PsiPort Browser – Quickly Check Analysis Results via the Web Browser

To achieve throughput improvements for synthesis researchers, it is important to simplify PC operations prior to starting analysis, and to make it easy to verify the acquired analytical data.

With PsiPort Browser, the Data View screen is provided for checking results via the web browser, allowing access to all the necessary information without performing complex operations.

This screen features a simple and easy-to-view arrangement. For example, a diagram of the sample rack with all of the registered vials is displayed, so that the analytical results associated with an individual sample can be obtained by simply clicking on the corresponding vial in the diagram. Likewise, clicking on a peak in the LC (UV/PDA/ELSD, etc.) chromatogram will display the corresponding mass spectrum, and vice versa. By setting the chromatogram / spectrum display parameters beforehand, the number of detected peaks and peak area values, etc. can be displayed. When output of the analytical results is desired, this screen can either be automatically printed as is, or it can be easily saved as a PDF file if Adobe Acrobat is installed.

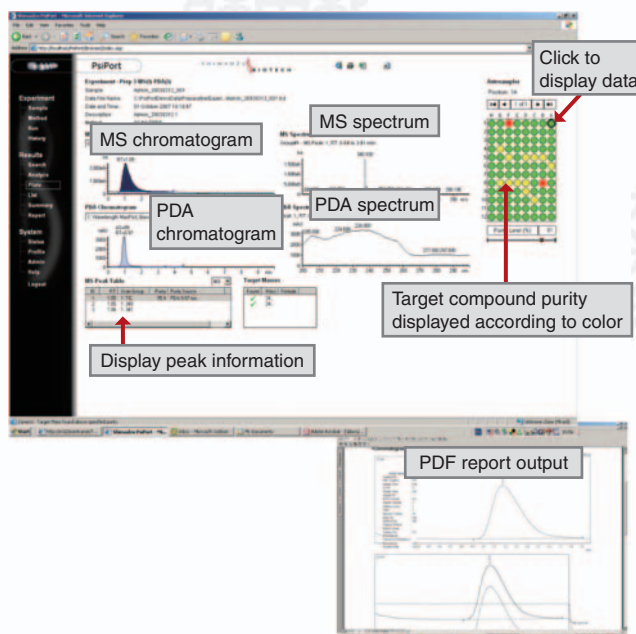


Fig. 3 Web Data Display Screen using PsiPort Browser

5. Merging of E-Mail and Web Browser – Hyperlink makes data search unnecessary

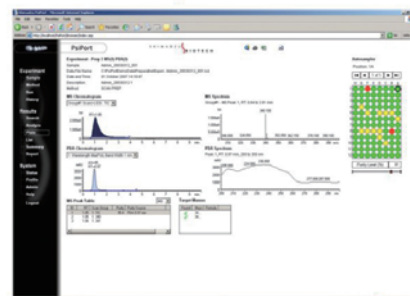
It is difficult to say that throughput can be improved by merely providing the ability to easily check analytical data.

It may be necessary to locate target data files of previous intermediate stages from a quantity of analytical data in order to adequately verify the content of an analysis. If this turns out to be a laborious task, there is a risk that any efficiency gains achieved up to that point might be wasted. One idea is to fully utilize the search function of Windows, but since this has functional limitations, time might be unexpectedly wasted. In order to further improve overall analytical efficiency, PsiPort Browser is equipped with hyperlink functionality as standard to easily access target data.

As an example, an e-mail that informs to the researcher that analysis is complete can be automatically sent and since the URL at which the analytical results are stored is included in the message, merely clicking on that link will display the analytical data in the web browser itself. Operations from analysis to data verification and output can be conducted stress-free in a short period of time – indicating that PsiPort Browser will liberate LCMS to all researchers.



Data search is necessary
→ Link directly to data



Perform all operations from your quarters

↓
No need to go to the lab

Fig. 4 Flow from Analysis Completion to Data Viewing

6. Schedule Editing – Easily accomplished by importing Excel Spreadsheet

PsiPort Browser also supports the ability to set up a typical multi-sample schedule for microplate (MTP) analysis.

PsiPort Browser comes equipped with the PsiPort Excel Wizard, enabling easy creation of schedules. By effectively utilizing this function, schedules created and stored on the PC in your quarters can be accessed and loaded using the lab-based instrument PC via the network.

Thus, all that is required to do in the lab is to read in the schedules and click the mouse button a few times.

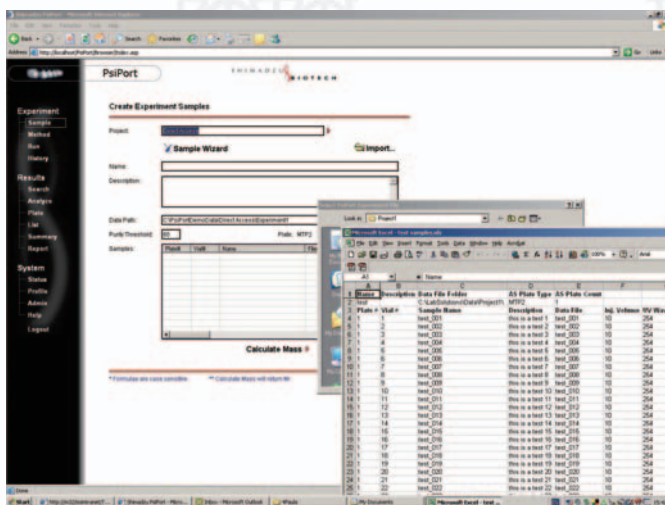


Fig. 5 Sample Registration via Excel Spreadsheet

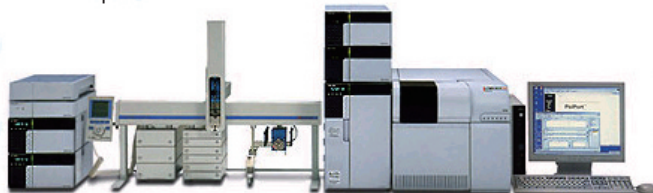
7. PsiPort Instrument Control – Enabling Further Open-Access Analysis

Whether you use vials or microplates, PsiPort can process, and track your results. Different sample processors, including Gilson's Liquid Handler and CTC's HTS PAL, were developed specifically to address flexibility in terms of sample containers.

PsiPort Browser supports both of these autosamplers, and the use of PsiPort Instrument Control provides the functionality to create the associated methods and perform instrument control. As a result, the work involved in exchanging vial and microplate racks is very simple.

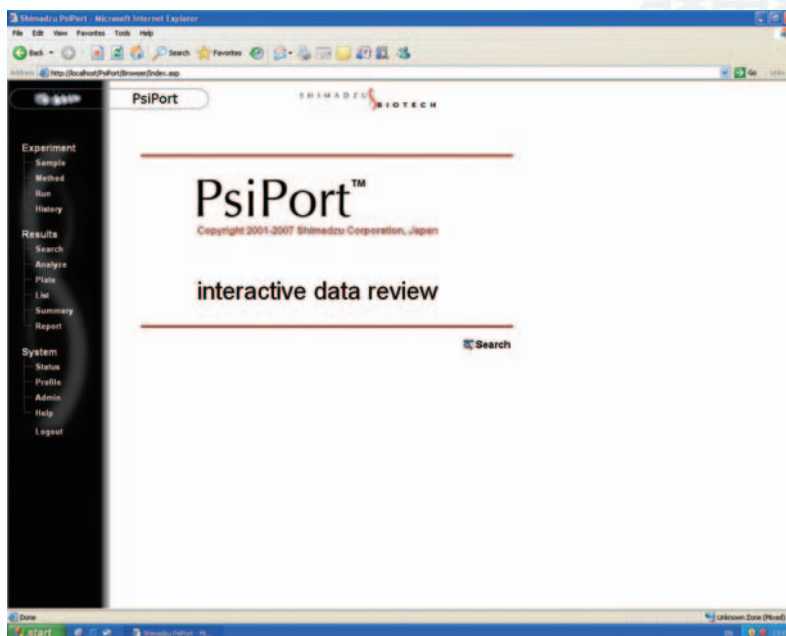


Gilson Liquid Handler



CTC HTS PAL

Fig. 6 PsiPort Instrument Control Application Examples



(Note) Windows, Internet Explorer, and Excel are registered trademarks of Microsoft Corp.

(Note) Please contact Shimadzu for information regarding supported equipment and software, and any necessary software that must be purchased separately.

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