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Applikationsbericht

Waters SDMS Vision Publisher - Recording an LC-MS Experiment

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Abstract

Waters SDMS Vision Publisher provides a reliable, easy-to-use, compliant-ready data storage, and retrieval tool for any scientific workplace that wants to manage information in a whole new way to increase productivity.

Introduction

Maintaining a paper research laboratory notebook is a tremendous amount of work, especially in today's data-rich research environment. It is estimated that researchers spend between 15 and 20% of their designated research time maintaining a paper notebook. The resulting notebook consists of a mixture of handwritten text and drawings and often becomes bloated with taped-in data hard copies. Unfortunately, depending on the handwriting and organizational skills of the scientist maintaining a notebook, the entries may only be legible or understood by the author. Furthermore, once a notebook is completely filled, it is often placed in storage or a library and it is not readily accessible for data retrieval. Hence, previously performed experiments within a laboratory are often repeated as there are no clear records of the methodology or experimental conditions. It is often easier to repeat the experiment rather than to find the original notebook entries.

With Waters SDMS Vision Publisher, scientists can electronically create, calculate, search, monitor, and report any type of scientific information. SDMS Vision Publisher addresses many critical workflow issues including improved productivity, information tracking, and intellectual property management. For capturing data, SDMS Vision Publisher is facile; there is no need to archive paper copies of tables, graphs, structures, chromatograms, spectra, or photographs, thus saving time and ensuring consistent recordkeeping. These digital forms of data can be captured either by the operating system clipboard, or by configurable instrument agents. Even multimedia files can be incorporated into an entry. Text, data, and calculations can be input using standardized business and data processing tools such as Microsoft Word and Excel, Waters Empower and MassLynx software, and more. Chemical structures can be drawn by using commercially available packages.

The advantages of using these programs are:

- entries are legible by multiple users
- entries can be standardized for the use of templates
- entries are fully searchable.

For example, entries can be searched within the text body, or by the use of metadata entries. Chemical structures can be searched by both full and substructures, as well as metadata descriptors. Hence, previously performed experiments can be found with ease on a laboratory or enterprise-wide scale. Finally, Vision Publisher comes 21 CFR Part 11 compliant-ready. These numerous capabilities are demonstrated in this application note, where a typical LC-MS experiment is conducted showing the creation of SDMS Vision Publisher entries, searching entries, and digital signatures features.

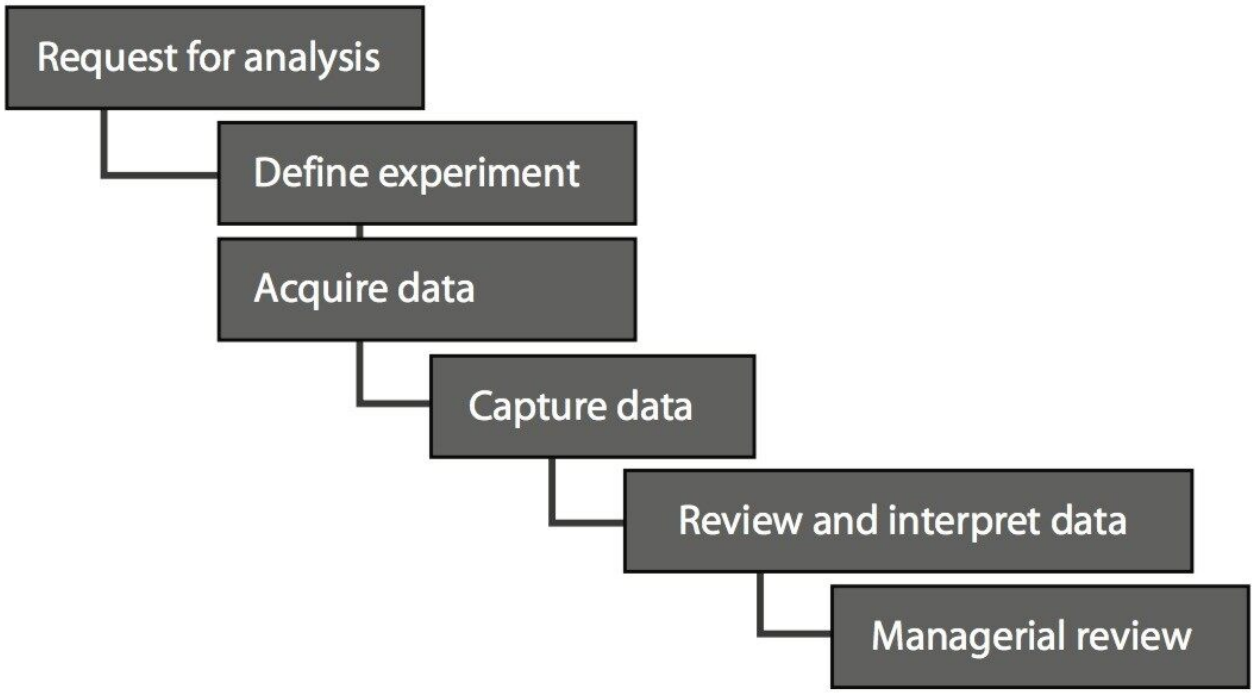

Figure 1. SDMS Vision Publisher manages the entire experimental workflow - data capture, data review, and storage.

Experimental

Simplify the Recording of Experimental Conditions

Once a new experiment begins, Vision Publisher allows you to capture all of the data elements that you would typically see in a paper notebook. Just as you would write your experimental aims and conditions, Vision Publisher allows you to digitally enter the same information with software programs that you already

use on a daily basis. In Figure 2 below, the Introduction and Experimental sections have been generated as notebook “objects” via input from Microsoft Word and Excel, with each new entry conveniently indexed on the left side of the page. In this case, Word was used to enter the textual components of the introduction and experimental sections, and Excel was used to capture the HPLC gradient table conditions.

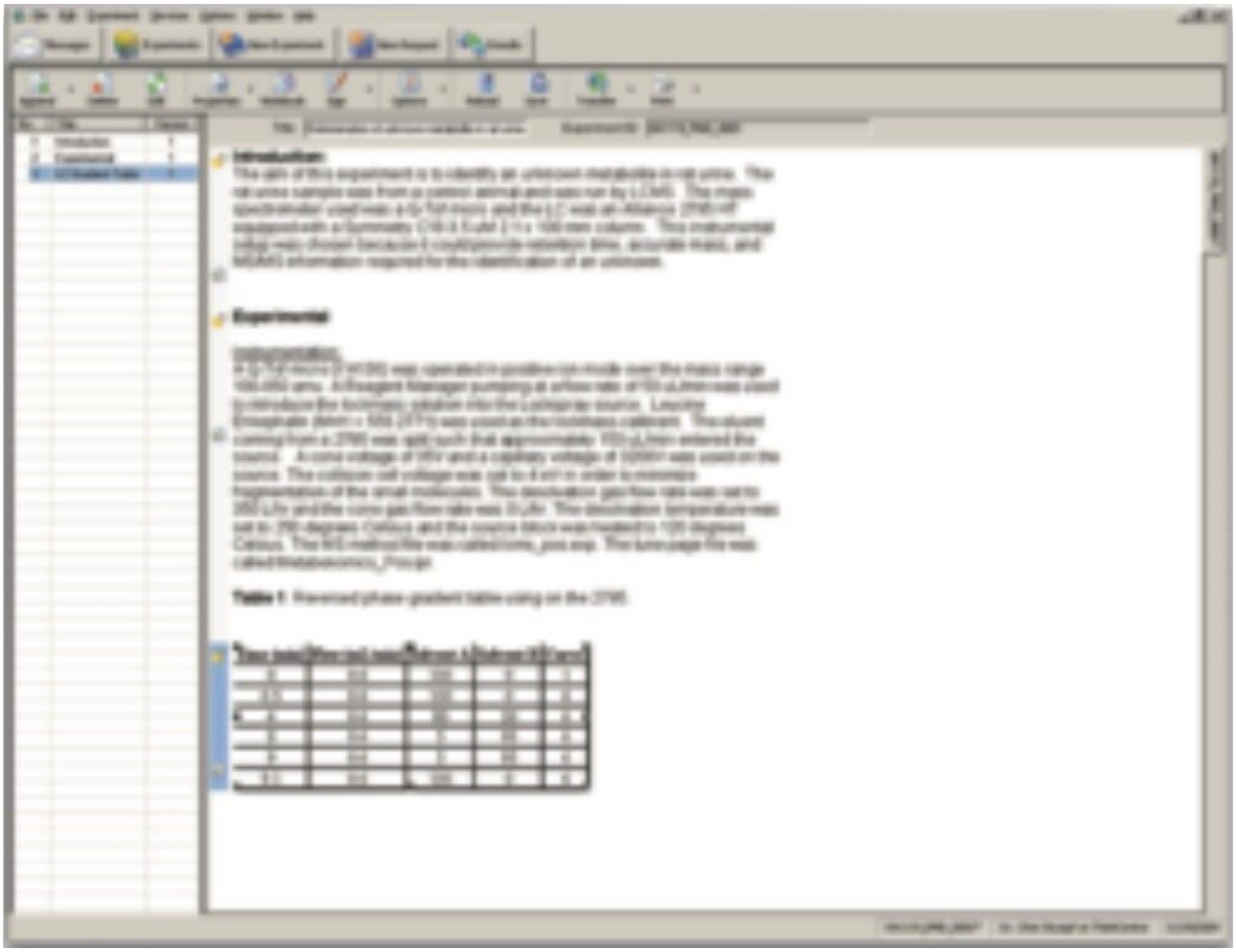

Figure 2. Vision Publisher entry illustrating the capture of the Introduction and Experimental sections of an LC-MS experiment from Word and Excel.

For full Vision Publisher interactivity with experimental detail, the text content of both the Word and Excel entries can be dynamically searched by using a full suite of search options. By making use of keyword metadata fields, more descriptor information can be applied to the information entered, and used for subsequent searches. The combination of these input and search functionalities is crucial to the day-to-day operations of research and discovery laboratories, as experimental information from related studies is often required for consistency of analyses.

Results and Discussion

Advanced Data Capture Tools

This process of manually cutting and pasting data hard copy into paper notebooks takes time, and paper copies often fade or become lost from the notebook. In contrast, when using Vision Publisher, the instrumental data can be copied and pasted directly from various data software packages. This operation can be performed in seconds, and becomes part of the permanent experimental record. An example of this procedure is shown in Figure 3, where the mass spectra of cholic acid are captured from MassLynx and copied into Vision Publisher's entry page. In addition, the use of corresponding metadata input makes the mass spectra searchable. The chemical structure of cholic acid is also shown in the Vision Publisher entry in Figure 3; this was drawn by using common structural drawing software (in this case, MDL ISIS/Draw), and then the structure was saved as an MOL file. An automated protocol was used to capture the MOL file into the "Results" section as a Vision Publisher object complete with an index entry. The advantage of using this method is that any future reference to this chemical entity (cholic acid) can be auto-populated for subsequent Vision Publisher entries and it is searchable as a full structure or substructure. The search results are displayed as a comprehensive table containing the structures found and active links to the corresponding experiments. Thus, this feature provides additional capabilities to enhance information management and retrieval.

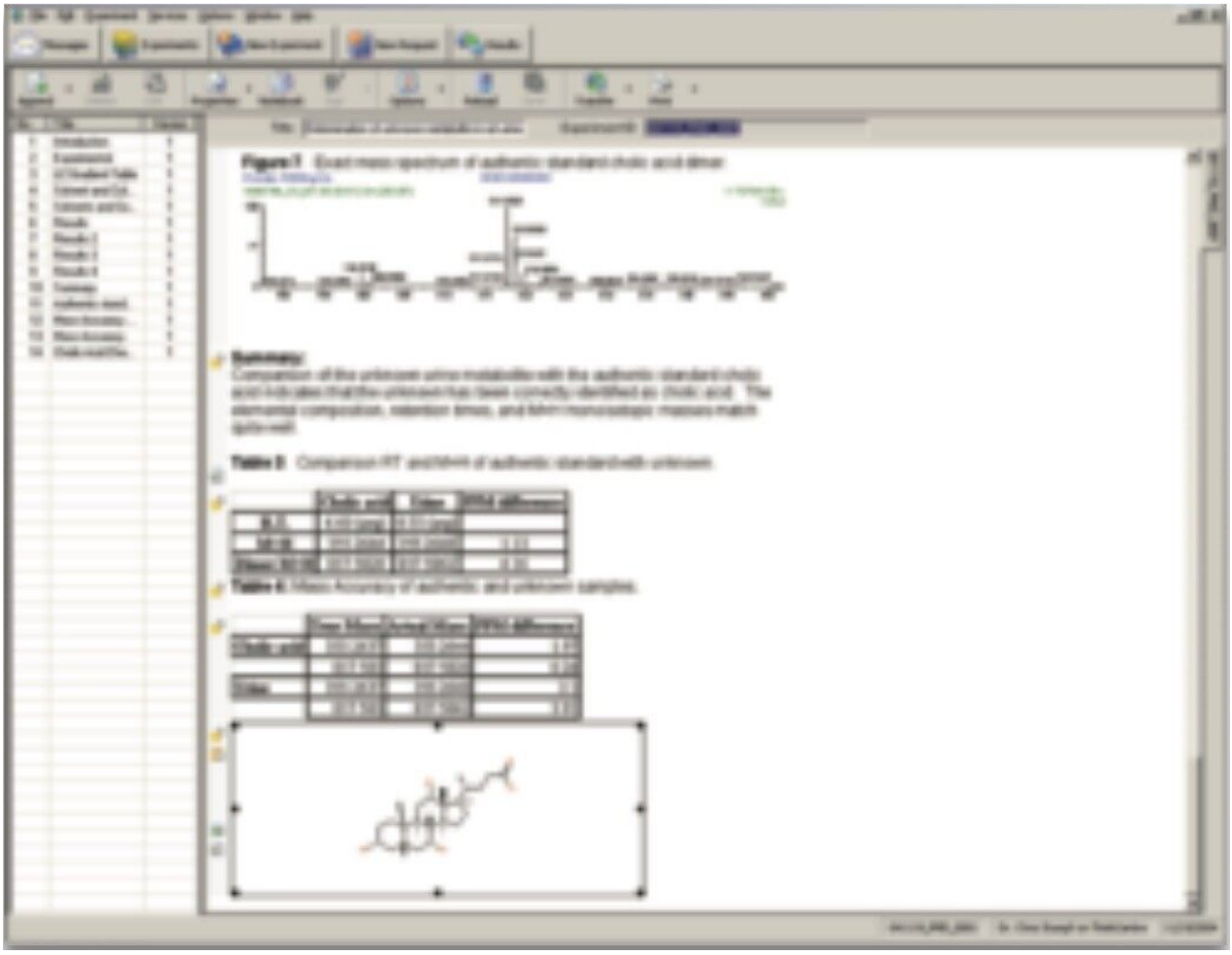

Figure 3. Vision Publisher entry showing the mass spectra and chemical structure of cholic acid.

Streamlining the Review Process

The U.S. FDA's 21 CFR Part 11 describes the criteria for the acceptance of electronic records and electronic signatures which are applicable to a wide range of FDA regulated industries. This regulation establishes the criteria under which the FDA considers electronic records and signatures executed to electronic records to be trustworthy, reliable, and generally equivalent to paper records and handwritten signatures executed in paper notebooks and documentation. SDMS Vision Publisher is 21 CFR Part 11 compliant-ready with statusbased user access, configurable electronic signature hierarchies, full audit trails, and digital signatures. The electronic signature protocol consists of all of the necessary descriptor elements such as author, experiment ID, signer, and reason for signature. Electronic signatures are made by authorized users with logins and passwords. This simple function is carried out with an email messaging system, which alerts various team members of upcoming action items generated within the Publisher entry, such as request for

signature and approval, and then it archives follow-up actions. This is particularly useful for laboratory managers, allowing them to follow the real-time status and compliance activities of the laboratory.

Figure 4. Example of the electronic signature process for Vision Publisher.

Comprehensive Audit Trail Information

A typical notebook entry consists of many sub-entries. Each of these sub-entries is monitored for changes as a record is maintained over time. The status of the overall notebook entry is monitored for any subsequent changes after approval. Vision Publisher uses secure, software-generated, time-stamped audit trails (Figure 5) to independently record the date and time of operator entries, as well as actions that create, modify, or delete electronic records. If a valid change needs to be made, it would be handled just as it would be in in a paper notebook, where the changed entry is appended to and witnessed and recorded electronically instead

of on paper.

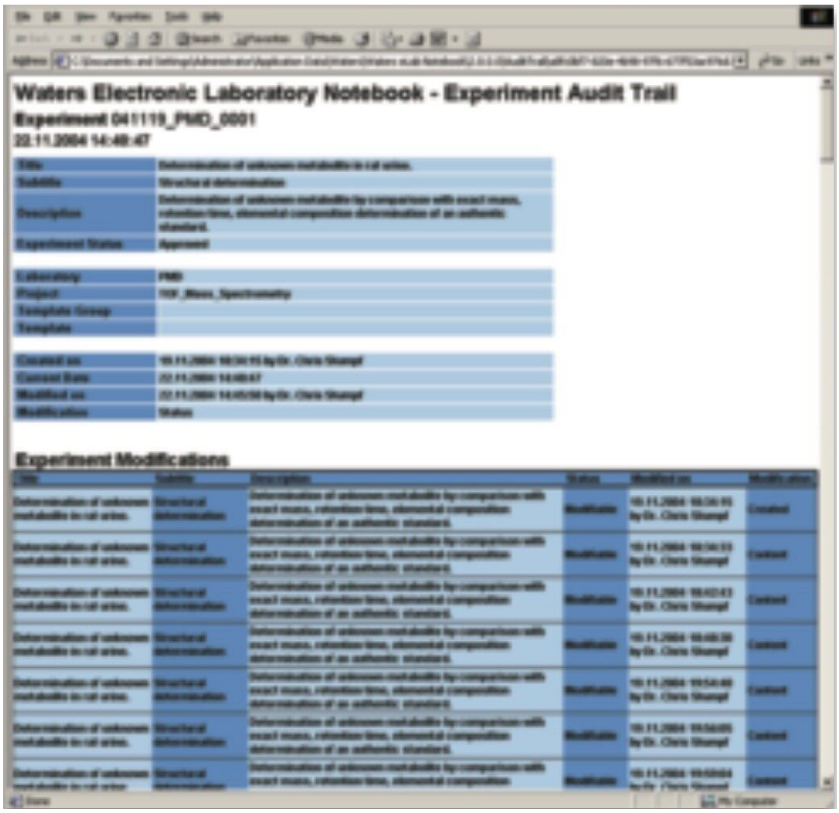

Figure 5. Audit trail for a typical Vision Publisher entry.

Conclusion

Waters SDMS Vision Publisher provides a reliable, easy-to-use, compliant-ready data storage, and retrieval tool for any scientific workplace that wants to manage information in a whole new way to increase productivity. Added functionality such as faster search capabilities and real-time messaging, enhance the data entry and review processes, so that more truly useful information can be mined across the organization.

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