

SDMS VISION PUBLISHER FACILITATING MASSLYNX AND EMPOWER SOFTWARE DATA CAPTURE

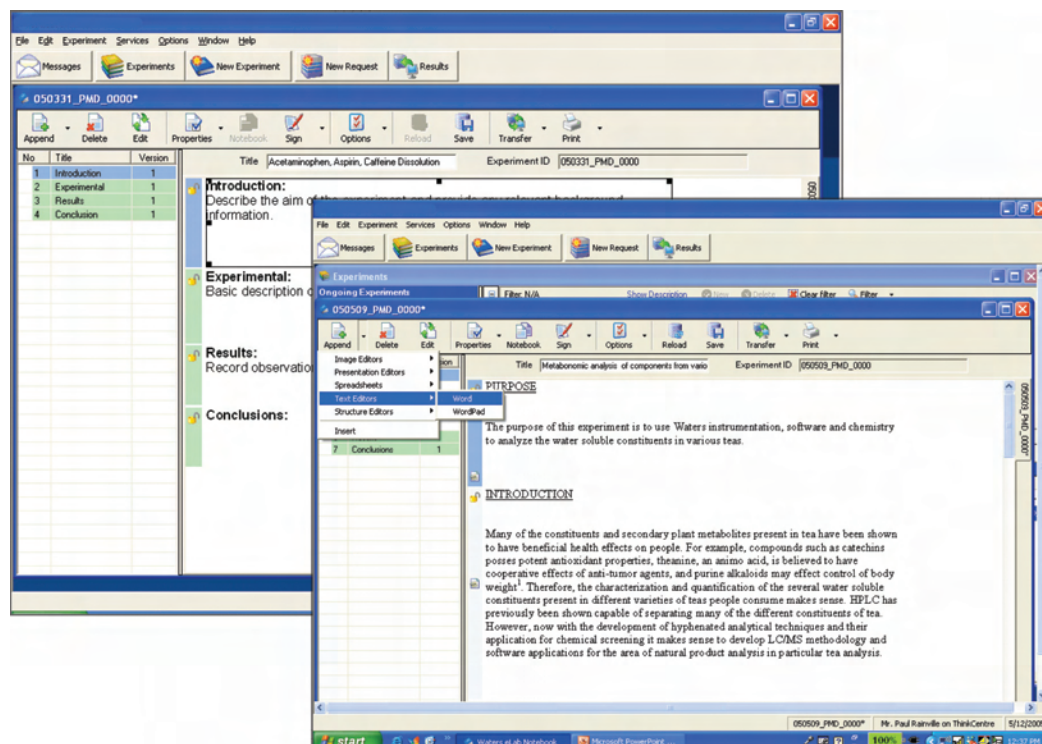
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Waters Corporation, Milford, MA, USA

INTRODUCTION

As the volume and complexity of research data continues to grow, the use of an electronic format for laboratory record keeping is the key to simple recording and global communication of critical scientific information. It is well known that this medium offers benefits over traditional paper-based notebooks as it requires less physical storage space, provides faster and easier search capabilities, and graphic and text-based information is easily captured without transcription error. Thus, experimental details can be recorded in an efficient, legible manner to create a shareable and searchable

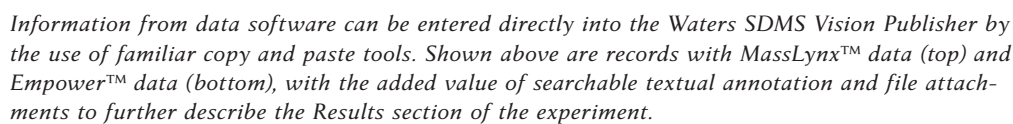
environment for present and future use. As the networking of laboratories becomes commonplace in many organizations, researchers require new means to organize and comprehend results. Keeping pace with advances in the Waters® Informatics portfolio of solutions, Waters has developed the Scientific Data Management System (SDMS) Vision Publisher to seamlessly interact with existing data products for streamlined usability and maximum productivity in a secure environment.

SETTING UP A PROJECT AND ENTERING INTRODUCTORY TEXT INFORMATION



Creating a new project in the Waters SDMS Vision Publisher. A unique numerical identification record is generated for each discrete experiment. Within a new record, standard word processing tools (such as Microsoft Office) are used for entering textual information. Pre-defined templates can be created to tailor for specific tasks and pass/fail criteria.

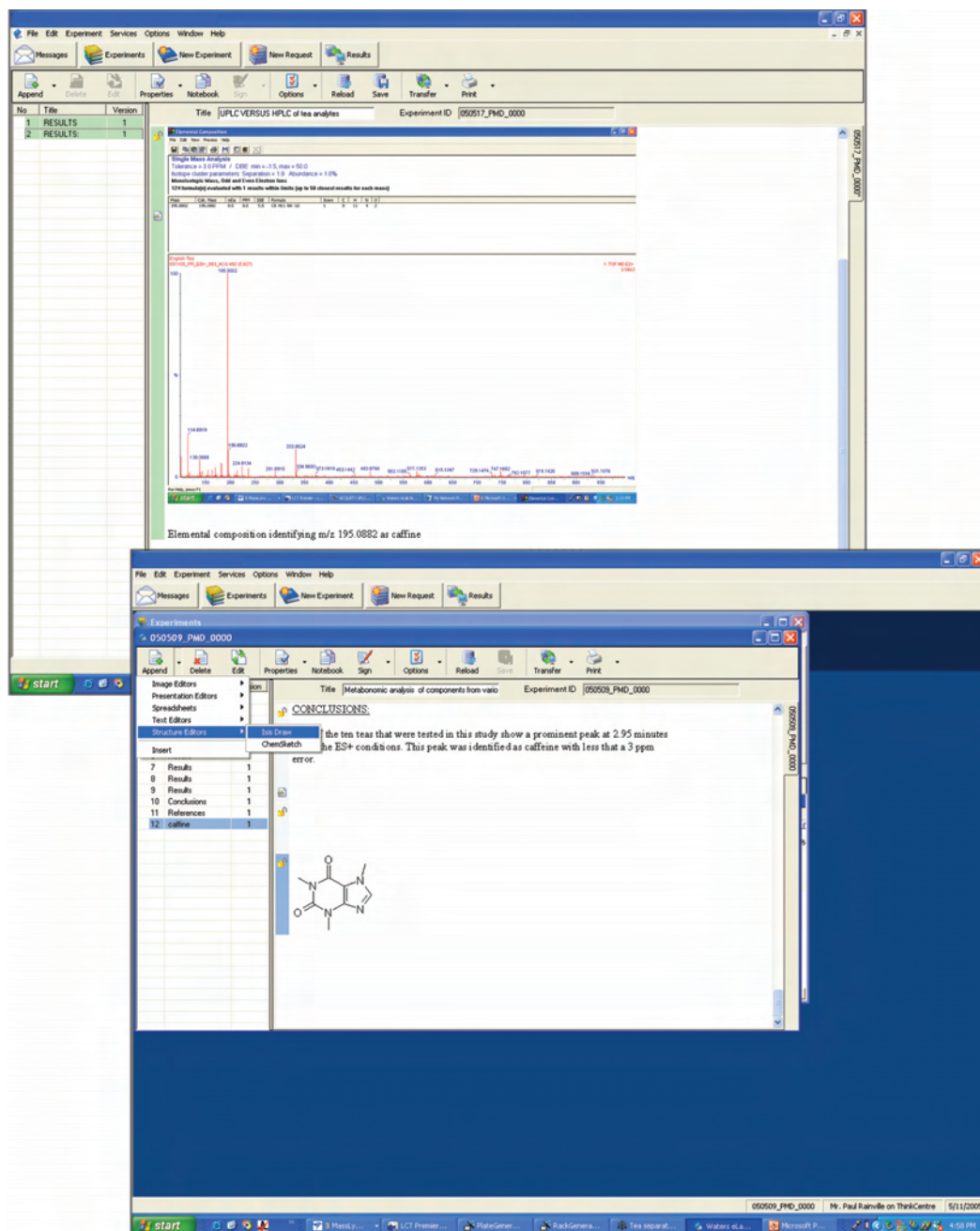
MASSLYNX AND EMPOWER DATA CAPTURE AND ANNOTATION



[APPLICATION NOTE]

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MASSLYNX DATA CAPTURE AND STRUCTURAL INFORMATION



MassLynx exact mass data is complemented by the ability to add searchable structural information. Here we show elemental composition (top), and corresponding molecular structure (bottom). Structures and sub-structures can later be searched across the entire Vision Publisher and displayed as a comprehensive table with active links to individual experimental records.

[APPLICATION NOTE]

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ELECTRONIC SIGNATURES AND FULL AUDIT TRAIL CAPABILITIES

The top screenshot displays the 'Release: RESULTS' dialog box. It includes fields for 'Entry Signer', 'Need Signer', 'Deadline' (set to 5/04/2005 2:41:54 PM), 'Priority' (set to Low priority), and 'Additional Notifications'. The 'Additional Notifications' field contains a list of names: Mr. Paul Raimale, Mr. Mike Jones, and Dr. Chris Stumpf. The 'Release Entry(s)' button is visible at the bottom.

The bottom screenshot shows the 'Experiments' list. The list has columns for Experiment ID, Title, Subtitle, and Description. The list contains four entries:

Experiment ID	Title	Subtitle	Description
050504_PMD_0000	Random UPLC Method Development	using Dyalab	Method development UPLC
050508_PMD_0000	Metabonomic analysis of components from soil	Metabonomic profiling of natural products	Analysis of different teas
050517_PMD_0000	UPLC VERSUS HPLC of tea analyses		
050517_PMD_0001	LCT Publication		

The 'Configure the audit trail content' dialog box is open, showing checkboxes for 'Experiment metadata', 'Experiment comments', 'Experiment links', 'Experiment content', 'Entry metadata', 'Entry comments', and 'Entry links'. The 'Experiment content' checkbox is checked.

Vision Publisher entries are signed electronically (top). Authorized approvers are designated from a pre-populated list of qualified individuals. Notification that signatures are required can be accomplished through the use of messaging capabilities with a specific date as to when entries should be endorsed. Full audit trails are also available if required by the organization (bottom).

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CONCLUSION

The recording, storage, approval, and retrieval of laboratory data is simplified and streamlined with the Waters SDMS Vision Publisher as an open interface for scientific documentation, safekeeping, and communication in the laboratory. It allows researchers to readily capture text, tables, spreadsheets, images, chemical structures, spectra, chromatograms, and many other data types in a single, digital environment. The increasing trend for laboratories to carry out research across multiple sites requires organizations to expand their data sharing capabilities beyond paper, while retaining the usability of traditional record keeping for day-to-day entries.

We have demonstrated the use of the Vision Publisher with MassLynx and Empower Software, highlighting the ability to interact with standard data software packages with straightforward cut and paste functionality, pre-defined templates, and common desktop tools to record experimental details and annotations, thus making it a state-of-the-art product that is readily adaptable to any laboratory workflow.

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March 2007 720002049EN JH-PDF

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