Waters

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NuGenesis SDMS Scientific Information Management Platform

Waters NuGenesis Scientific Data Management Software (SDMS), a key offering in the Waters Laboratory Informatics (WLI) Suite, is an application-independent software and database platform that is used to create a common electronic repository for scientific information throughout your company. Using sophisticated database technologies to capture, store, and retrieve scientific information, the Waters NuGenesis SDMS lets you focus on science by eliminating the paper and data file back up burden. Technologies from Waters end the hunt for paper-based data and eliminate countless hours of cutting and pasting information into reports, presentations, and other types of submissions while also providing a secure, compliant-ready repository for scientific data files.

Waters NuGenesis SDMS improves the value of information by enabling scientists to unify, share, and fully reutilize scientific data generated from the vast array of laboratory applications. WLI products provide scientists, from the bench to corporate management, with unique capabilities such as compound document creation, immediate electronic online access to different types of laboratory information, accelerated electronic submissions, improved document preparation, enhanced patent protection capabilities, and seamless integration of data with LIMS packages.

NuGenesis SDMS Software V7.0 Introduction

The NuGenesis SDMS V7.0 release builds upon the success of the SDMS V6.0 platform. Through the inclusion of new platform architecture, administration and end user features, users enjoy greater deployment and user flexibility. This makes it easier for organizations, small and large, to realize the benefits of this comprehensive data repository. We have also extended the "plug and play" nature of the architecture to make it easier to add features with minimal validation and deployment impact. As the first SDMS release as part of Waters Laboratory Informatics, it also includes even tighter integration with other WLI products, including Waters eLab Notebook, Empower and MassLynx, providing clear benefits to Waters customers.

NuGenesis SDMS 7.0 is based on an Oracle 10g database, providing higher performance and added enterprise management, backup and recovery tools. Protecting and preserving data is a fundamental design requirement of the repository. Thus, it has been enhanced with additional data verification checks to further safeguard your critical data. The new managed storage option provides additional flexibility in system architecture, storing files on a designated share (typically a SAN or RAID) as an alternative to inside of the database. This allows systems to be configured to make the best of existing network infrastructures. The system supports single user authentication strategies through support of Active Directory and other LDAP technologies and includes new web based administrative tools for user/group management and remote server monitoring and management.

Previous versions of SDMS included extensive capabilities for searching, viewing and mining of point in time results or print data. SDMS V7.0 has enhanced these capabilities for raw or file data. New Data Adapters (formerly called Enhanced Vendor Support (EVS) modules) for Microsoft Office and Adobe .PDF documents fully index all text in these files, allowing them to be easily searched and located. Data Adapters for scientific data include automatic conversion capabilities that create JCAMP-DX public data standard files. These enable viewing, mining and long term preservation of active scientific data. The new analytical data viewer provides for viewing of a variety of commonly used data in JCAMP-DX format such as optical spectroscopy, NMR, MS, chromatography, hyphenated methods, and chemical structures, right on your computer desktop—without the original application.

Facilitating the re-use of the data in the SDMS repository for end users and for integration applications is another design target for SDMS V7.0. All users routinely interact with the VISION browser, which has been redesigned for ease of use and performance. The Preview application for viewing, comparing, annotating and signing of print data includes new buttons and usage properties that simplify electronic signature and other collaboration processes and move with the user in cases where they work on multiple PCs. The configurable extraction templates and the Software Development Kit (SDK) now include capabilities to configure the automatic extraction of graphic elements from print data for use in other data analysis or viewing applications. The SDK documentation also includes instructions for using standard

Microsoft tools to create .NET compatible SDK applications in addition to continuing the Microsoft Active X and Java support.

New Features in NuGenesis SDMS 7.0

1) System Architecture

a) Platform Support-

SDMS Component(s)	Validated Operating Systems, Browsers and Databases				
Web Application Server	Windows Server 2003 SP1 with IIS 6.0, Windows 2000 SP4 Server and				
	Professional with IIS 5.0, New Atlanta ServletExec 5.0.0.10, Java ™				
	Runtime Environment Standard Edition 1.4.2.08				
SDMS VISION Browser including	Windows Server 2003 SP1, Windows XP SP2 Professional, Windows				
Preview (print data viewer),	2000 SP4 Professional & Internet Explorer 6.0				
Restore (file data restoration) and	** Internet Explorer 6 is not supported on Apple Mac OS X, therefore				
Analytical Data Viewer (JCAMP-	none of these web based applications will operate on the MAC OS X				
DX data viewer)					
SDMS Help Desk					
SDMS Remote Server Console					
SDMS Administrator	Windows Server 2003 SP1, Windows XP SP2 Professional, Windows				
UNIFY Print Capture Modules	2000 SP4 Server and Protessional				
SDMS File Capture Modules					
Jukebox Engine	ArchiveXtender V5.1 software from EMC/Legato on Windows Server				
	2003 SP1 and Windows 2000 SP4 Protessional and Server.				
Oracle Server	Oracle 10.1.0.4 Server on Windows Server 2003 SP1				
	Oracle 10.1.0.4 Server on Windows 2000 SP4 Server				
	Oracle 10.1.0.4 Server on HP UNIX Version 11				
	Oracle 10.1.0.4 Server on Sun Solaris UNIX Version 9				
	Oracle 10.1.0.4 Server on IBM AIX 5.2				
Oracle Client	Oracle 10.1.0.3 Client for Windows XP SP2 Professional, Windows				
	Server 2003 SP1 and Windows 2000 SP4 Professional and Server				
User Identity Servers supported	Microsoft Active Directory on Windows Server 2003 SP1 or Windows				
for authentication					
	Sun iPlanet Directory Server VS.1 Service Pack 2				
Data Source Operating Systems	Microsoft Windows NI 4 SP6a, Microsoft Windows 98 SE, Windows				
for File Data	2000 SP4 Professional, Windows XP SP2 Professional, UNIX (via				
	SAIVIDA OF VVINGOWS SERVICES FOR UNIX 3.5 gateway software) and				
	Apple maciniosin US A 10.2 (via FC/MACLAIN V9 gateway software)				
Lata Source Operating Systems	vvindows 2000 SP4 Protessional, vvindows XP SP2 Protessional, UNIX				
TOR FRINT DATA VIA UNIFT PRINT	and Apple MAC US X 10.2.3 (through NuGenesis UNIF (ps)				
Modules					

b) Multi language support- supports use in English, French, Italian, German, Spanish, Japanese environments for data and user entered content.

c) The Managed storage option allows projects to be configured such that data is stored on shared FTP location as an alternative to storing the data in the database. This provides deployment flexibility and allows for configurations that will dramatically decrease network traffic, especially needed for customers managing large files such as images. It also is the preferred configuration from a performance perspective for systems managing high volumes of data or managing large data files.

- d) The Offline Storage Manager includes a new HSM Store archive device. This logical device is designed to be used with SAN and Network Appliance storage devices that are serviced by commercially available Hierarchical Storage Manager systems.
- e) Support of Oracle 10G client and server-adoption of these database components will provide long term platform stability (~3 years) and adds improved performance and new enterprise management tools included validated back up and recovery scripts using Oracle Recovery Manager (RMAN).
- f) Compliance with the correct number of purchased licenses is ensured through the enforcement of named user license quantities by the system.
- g) Installers for the most commonly distributed software modules have been enabled to support silent installation through IT tools such as Microsoft Systems Management Server (SMS). These include SDMS Administrator, VISION Transfer Application and the Web based UNIFY Print Driver.

2) VISION

a) Updated User Interface- The VISION browser continues to be based on a familiar spreadsheet-like view of the data catalog. Navigation has been simplified through the inclusion of more buttons and menus while eliminating unnecessary mouse clicks.

1) Simplified Project Tree: The Print Data and File Data tree nodes have been removed; projects are now listed alphabetically with appropriate icons to designate the project type.

2) File Data View Extended Details page converted to a table view to present more information without the need to scroll.

- b) Analytical instrument and many other types of files can be viewed directly from the VISION browser through a single mouse click using the viewer(s) provided with SDMS, or those supplied on your PC.
- c) View, annotate and share data from NMR, MS, UV/Vis, chromatography, hyphenated methods, chemical structures and other techniques through the Analytical Data Viewer and the new public data standard conversion capabilities.
- d) MassLynx Application Manager Browser Support- The OpenLynx, QuanLynx and FractionLynx browsers can be launched directly from Vision when their respective files are selected.
- e) Expanded yet simplified search capabilities make finding data easier

1) Text from Microsoft Office (Excel and Word) and Adobe portable document format (PDF) files can now be used to search for these files.

2) New Find Related Data search automatically uses common metadata to logically connect any data in the SDMS repository. This is ideal for linking print data to related file data through the data model.

3) View filters now support date math to be able to a specify date selection based on 28 relative date functions such a CDATE, LMONTH, WEEK and MDAY. This is particularly useful for administrators that want to calculate metrics. For example, to select all records that are older than 180 days a filter of <=CDATE()-180 would be used.

f) Annotation and Electronic Signature tools have been expanded to include new buttons and most recently used settings for items such as placeable annotations. This lowers user acceptance barriers by making it easier to implement review and signature processes electronically.

3) Administration

- a) The SDMS Help Desk is a new web based administration module for users, groups and privileges, targeted for use by corporate help desk departments.
- b) The SDMS Administrator has a number of ease of use and operational enhancements.

1) The tiered administration model includes additional privileges to make it easier to configure administrative and user groups and activities while restricting access to high level server based features.

2) Administrators can now print Tag Lists, User Lists, Group Lists, Global Privilege Lists and Project Privilege Lists.

- 3) The Privilege grid locks and scrolls to make it easier to manage complex privilege settings.
- c) Search Groups is the new administrator tool for configuring the "Find Related Data" search. A Search Group is analogous to a high level group of Projects/Views. It links various records by mapping tag fields or metadata between various projects, taking advantage of the data model used for the capture of data. This map is then used to execute searches that locate records with the same metadata values. Typical applications of this feature would map tags between print and file data projects to make locating related data easier.
- d) The SDMS Remote Server Console is a web based tool for monitoring and managing SDMS File Capture server components. At the same time, it acts as a portal for access to tools such as the Oracle Enterprise Manager and the SDMS Activity Log project. The tool also provides summary information on selected server parameters.

4) File Capture Technology:

a) Several deployment and performance related parameters have been added to the file capture modules to provide additional implementation choices based on network infrastructure and desired performance.

1) The transport engine service includes a new scheduling feature to provide opportunities for managing network traffic. It allows the Transport Engine to be turned on and off once during each day, e.g. off at 8:00 am and then back on at 8:00 pm

2) The archive agent's scan cycle parameter has been reduced by a factor of 4, allowing it to be configured to scan data source locations more frequently.

- b) Administration of file capture templates has been improved through a new template builder user interface that includes new organizational tools such as sorting and comments. Additionally, new archive command line filters such as folder patterns can be used to decrease the number of command lines necessary for many common applications.
- c) The archive agent and corresponding Data Adapters (formerly called EVS modules) include new capabilities to provide for conversion of select data types into a public data standard. The well known JCAMP-DX standard is the technology neutral data format supported. Records that include this converted data can be viewed in VISION with the Analytical Data Viewer, as well as restored for use in their original application. Please refer to the application specific Data Adapter table for details on those adapters that support JCAMP-DX conversion.
- d) Earlier versions of the NuGenesis SDMS file capture architecture only supported file capture using a scan and pull model where the source location was scanned, then the file was pulled to the repository. It now supports the development of applications that will push file data into the repository while ensuring that the repository based features such as data management and restoration back to the original location are still available. Selected Data Adapters are "proxy enabled" such that they can receive files from these manual

archive applications while still allowing the tag marker mapping capability of the data adapter. The SDK includes new "Archive On Demand" application program interfaces (APIs) that are used to create these applications. Please refer to the application specific Data Adapter tables for details on those adapters that are proxy enabled.

e) A new HSM Store logical archive device selection has been added to the Offline Storage Manager (OSM) to enable configuration of an archive device that can be used in conjunction with third party hierarchical storage software. The HSM Store archive device operates identically with the RAID archive device but is treated as a single continuous volume that will never run out of space.

5) Data adapters

a) Data Adapters (formerly called Enhanced Vendor Support or EVS Modules) are plug and play modules that provide for the definition of the archive behavior and metadata extraction from file data. The two categories of data adapters are NuGenesis Generic and Application Specific. NuGenesis Generic adapters are a standard non-specific offering that can be used to capture any type of file data. The metadata extracted from these files is dependent upon the file system infrastructure and companion files generated manually or automatically by an external application. Application specific adapters include standard and optional offerings that are used to archive data from a specific application. The archive behavior and metadata extraction is specific for data generated by that software version. Since application specific data adapters often use automation tools in the specific application, they may require installation of that application on the file capture server, or installation of a remote data adapter on the machine running that application.

Vendor	Product/ Version	Data Element Type	File Pattern	Proxy Enabled	Comment
NuGenesis	Cascade Folder Template	File- based	* *	No	
NuGenesis	Generic	File- based	* *	Yes	
NuGenesis	Generic Macintosh	File- based	* * ·	No	
NuGenesis	Image OCR	File- based	*.* *.BMP *.DCX *.JPG *.JPEG *.PCX *.PNG *.TIF	No	Requires optional OCR Engine License
NuGenesis	Per File Template	File- based	* *	Yes	
NuGenesis	Per Folder Template	File- based	* *	No	

b) NuGenesis Generic Adapters

.* New or updated adapters are *blue*.

Vendor	Product/ Version	Data Element Type	File Pattern	Proxy Enabled	JCAMP-DX Conversion	Application Client Required	Product Technique
ABI-Sciex	Analyst 1.2-1.4	File-based	*.wiff	No	No	Yes	LC/MS
ABI-Sciex	Analyst 1.2-1.4	File-based	*.rdb	No	No	Yes	LC/MS
Adobe	Acrobat V 4.0- 7.0	File-based	*.pdf	No	No	No	Documents
Advanced Chemistry Development	ACD SpecManager/ ChromManager V 6.0-8.0	File-based	*.esp	No	No	No	GC, LC, GC/MS, LC/MS, NMR, MS, UV, IR, Curves
Agilent Technologies	Agilent Chem- Station ¹ 6.0,6.03,8.0, 9.0 and 10.0	Directory- based – Grouped by data folder or data with method subfolder	*.*	No	Yes for LC, GC, GC/MS and LC/MS data	No	GC, GC/MS, LC, LC/MS, LC- Photodiode Array (PDA)
Agilent Technologies	Agilent Chem- Store Client- Server V B.02.02	File based group : Archive Unit file and XML Catalog file	**	No	No	No	GC, GC/MS, LC, LC/MS, LC- Photodiode Array (PDA)
BD Biosciences	CellQuest Pro V5.0, FACSArray V1.0 and FACSDiVa V4.0	File-Based	*.FCS	No	No	No	Flow Cytometry
Brinkmann Inst.	Titrino Workcell, V4.0 and V4.5	File-based	* *	No	No	No	Titration
Bruker BioSpin	XWIN-NMR V3.0	Experiment Number based (multiple folders)	**	No	Yes for 1D NMR Data	No	NMR
Bruker BioSpin	XMASS V5.0	Experiment Number based (multiple folders)	**	No	No	No	LC/MS
Dionex	Chromeleon Sequences V6.6	Database based	**	No	Νο	Yes, uses remote adapter on source machine	HPLC, Ion Chromatography (IC), GC, LC, LC/MS

c) Application Specific Data Adapters.

Vendor	Product/ Version	Data Element Type	File Pattern	Proxy Enabled	JCAMP-DX Conversion	Application Client Required	Product Technique
Dionex	Chromeleon Samples V6.6	Database based	**	No	No	Yes, uses remote adapter on source machine	HPLC, Ion Chromatography (IC), GC, LC, LC/MS
MDL	Isis Draw	File-based	*.mol	No	No	No	Chemical Structures
Microsoft	Microsoft Office 2000, XP and 2003 Excel, Power Point and Word	File-based	*.xls, *.ppt, *.doc	Yes	No	Yes	Documents
Perkin Elmer	Turbo-Chrom V6.12 or Total- Chrom V6.2 Client Server or Work Station	File-based	*.rst, *.raw	No	No	Yes	GC, LC, LC-PDA
Scientific Software, Inc.	EZChrom Elite V2.61	File-based	* * ·	No	No	Yes	GC, LC, LC-PDA
Shimadzu	CLASS-VP V4.3 and V5.03-6.0	File-based	*.dat	No	No	Yes	GC, LC, LC
Shimadzu	Class 5000,	File-based	* * .	No	No	No	GC/MS
Thermo Finnigan Corporation	Chrom-Quest, 2.5	File-based	*.dat	No	No	Yes	GC, LC, LC-PDA
Thermo Finnigan Corporation	Xcalibur V1.2 RAW files	File-based	*.raw	No	No	Yes	LC/MS
Thermo Finnigan Corporation	Xcalibur V1.2 RST files	File-based	*.rst	No	No	Yes	LC/MS
Thermo Electron Informatics	Atlas 2000 and 2003 SR 1 Work-books	Work-book based (modified directory)	* *	No	No	Yes	GC, LC
Waters Corporation	FractionLynx 3- 4-4.0	File-based	*.fpt	No	Yes	Yes	LC/MS
Waters Corporation	MassLynx, 3.4- 4.0	Directory- based	* *	Yes	Yes	Yes	GC/MS, LC/MS
Waters Corporation	OpenLynx, 3.4- 4.0	File-based	*.rpt	No	Yes	Yes	LC/MS
Waters Corporation	Empower/ Millennium ³² V4.0 Network and Workstation Projects	Database- based ^{**}	**	No	No	Yes, uses remote adapter on source machine	GC, LC, LC/MS, LC-PDA

Vendor	Product/ Version	Data Element Type	File Pattern	Proxy Enabled	JCAMP-DX Conversion	Application Client Required	Product Technique
Waters Corporation	Empower/ Millennium ³² V4.0 Network and Workstation Injections	Database- based ^{**}	**	No	No	Yes, uses remote adapter on source machine	GC, LC, LC/MS, LC-PDA
Waters Corporation	Empower/ Millennium ³² V4.0 Network and Workstation Results	Database- based ^{**}	**	No	No	Yes, uses remote adapter on source machine	GC, LC, LC/MS, LC-PDA

.* New or updated adapters are *blue*.

- d) The new Empower Data adapter uses technology that simplifies deployment and configuration. This data adapter includes a remote module that is installed on the Empower/Millennium client machine or work station. This module is in communication with the file capture server during data management operations.
- e) Support for Waters MassLynx and its application managers has been expanded with 3 new data adapters: MassLynx Raw Folders, OpenLynx and FractionLynx. Configuring the system to capture MassLynx data has also been simplified with the new Folder Pattern feature of the file capture template. This allows a single command line to capture files from multiple MassLynx Project folders.

6) Print Capture Technology:

- a) The UNIFY printer can now capture more data from more applications and configurations through support of 49 paper sizes including: Letter (8 ½ x 11 in), Legal (8 ½ x 14 in), A4 (210 x 297 mm), A5 (148 x 210 mm), A3 (297 x 420 mm), B5 (JIS)(182 x 257 mm), B4 (JIS)(182 x 257 mm), 10 x 11 in, 10 x 14 in, 11 x 17 in, 6 ³/₄ Envelope, 9 x 11 in, A2 (420 x 594 mm), A3 Extra (322 x 445 mm), A4 Extra (9.27 x 12.69 in), A5 Extra (174 x 235 mm), B4 (ISO) (250 x 353 mm), B5 (ISO) Extra (201 x 276 mm), German Legal Fanfold (8 ½ x 13 in), German Std Fanfold (8 ½ x 12 in), Japanese Post Card (100 x 148 mm), Ledger (17 x 11 in), 16 types of envelopes and others.
- b) Several deployment and operation related features have been added to the print capture modules to provide additional implementation choices based on network infrastructure and desired user experience.

1) Each UNIFY printer can be configured to automatically re-authenticate after re-boot with an administratively configured user account.

2) Message logs generated by any of the UNIFY print drivers are automatically uploaded to the Activity Log project just as that of the file capture modules allowing centralized review and trouble shooting from the web.

3) Up to 32 UNIFY printers can be configured on each PC, with pre-defined or user selectable project and template selections to make capturing data from multiple applications easy. Each printer can be named separately making the application specific selection easy in either batch or manual mode operations.

4) UNIFY settings have been expanded to automatically provide checks that ensure reliable operation through the inclusion of the minimum disk space warning limits.

5) The UNIFY printer can be configured as a CITRIX printer allowing IT and validation strategies that employ Citrix Clients and Servers to be utilized.

6) The UNIFYps Post Script printer for use in capturing print data from UNIX and Apple OS X systems now operates as a service that will re-start automatically after a re-boot or power failure.

- c) Print Capture Templates include new features that allow for more choices in the definition of tags including the new derived values: Constant Value, Report Name, Printing Application Name.
- d) Extraction Templates can be configured for automatic extraction of graphic data. One or more graphic element can be defined for extraction. The graphic elements may be located based on an explicit rectangle, or relative to a marker as with print capture templates. The graphic element could consist of a full page, a section or sections of a page, multiple pages or multiple reports.

7) Preview (Print Data Viewing) Technology:

a) Preview includes many new features that make it easier for users execute electronic signature and other operations

1) Preview Options now include choices for printing of electronic signatures and notations after reports., and can be saved in the database on a per user basis so that they will be available to the user regardless of the machine they are using.

2) Annotation preferences such as the location, color and size of the placeable marker, can be saved and are available in subsequent operations.

3) Report annotations, electronic signatures and the overlay viewer now may be accessed from icons as well as the menu simplifying their selection and use.

b) The Overlay Viewer tool, introduced in SDMS V6.01 SR-4, for print data evaluation and collaboration, allows one to select areas within reports and overlay them on screen for comparison, now includes new operational and ease of use features. Overlay viewer options are stored as part of the preview options therefore move with the user. It also includes the capability to rotate layers, click on a "move to front" selection and improved slide show indicators. This is especially useful for spectral and chromatogram report comparisons.

8) Software Development Kit (SDK):

a) The SDK has been expanded and enhanced to better facilitate application development and performance in the areas of graphical extraction template usage, file capture, file restore and printer configuration The following new methods (Active X descriptions shown) including example code have been included in this release:

1) ApplyGraphicalExtractionTemplate – Call this method to apply a graphical Extraction Template to a report with a specified format and destination for the output.

2) ArchiveFiles - Call this method to archive data using proxy enabled data adapters.

3) GetAODSupportedEVSList – Call this method to get a list of the data adapter packages installed on the client machine that are proxy enabled.

4) GetProjectProperties - Call this method to determine if a project's properties are enabled or disabled.

5) GetRestoreLocationsList – Call this method to retrieve a list of available locations to use when restoring files.

6) GetTagLabelsAndAliases – Call this method to retrieve the tag labels and aliases for a working view.

7) Get UNIFYPrintersList – Call this method to retrieve a list of UNIFY printers installed on the client machine supporting application-specific printing.

8) RestoreFileGroups - Call this method to restore a list of file groups.

9) RunAuditViewer – Call this method to open the Audit Trail Viewer to display audit trail information tracked by the NuGenesis SDMS programs at the project and server level.

10) SetUNIFYPaperSize – Call this method to specify the paper size to be used when printing from a specified application.

11) SetUNIFYPrinter – Call this method to specify the UNIFY printer instance to be used before calling any of the SDK application-specific printing methods.

- b) The SDK documentation now includes instructions for using common Microsoft development tools to develop Microsoft .Net wrapper applications for various SDK objects in ActiveX.
- c) The SDK documentation now includes Scripting Control Help instructions for accessing NuGenesis SDMS functionality from within scripts.
- d) Restore has been restructured so that individual restore processes executed through the SDK can be executed and provide feedback directly to the calling application. This is especially useful developing applications that are restoring large numbers of files.