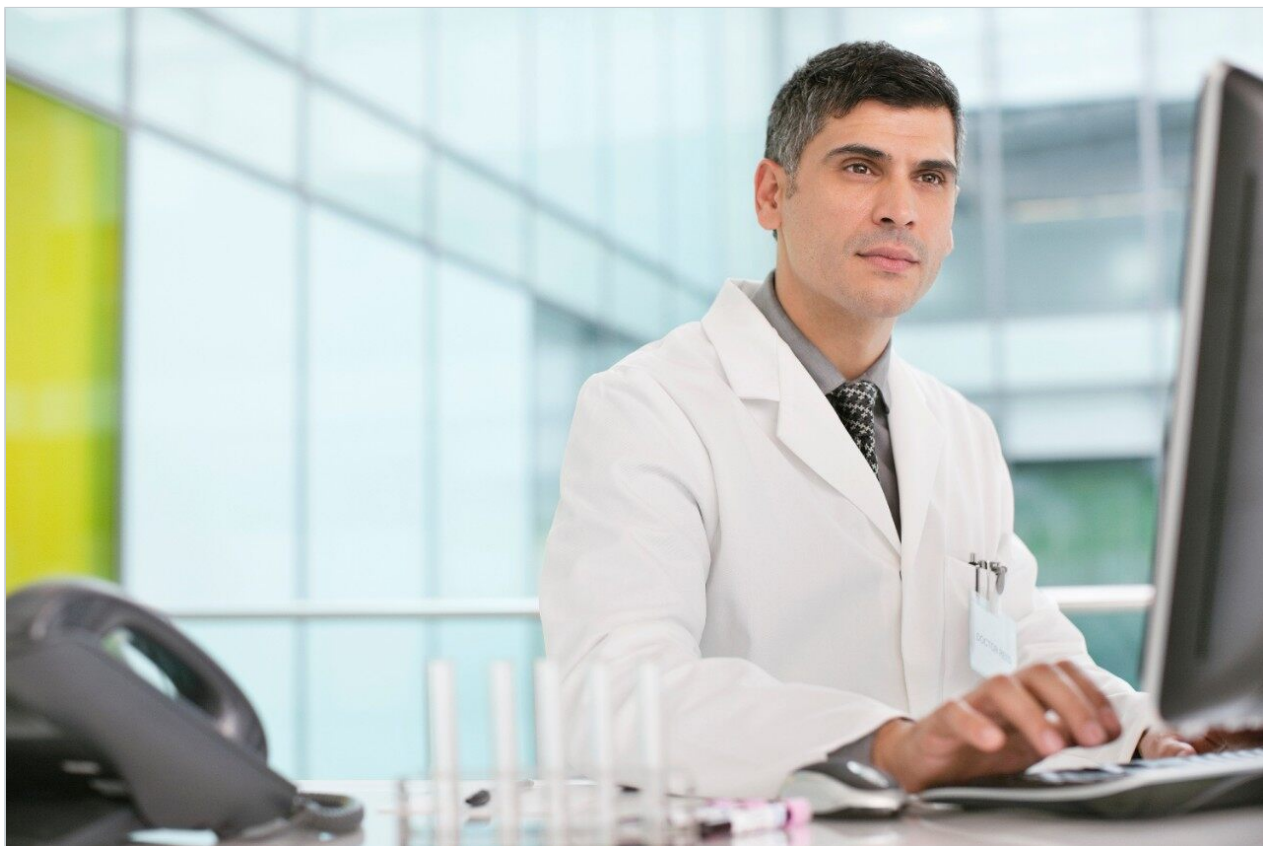


An Integrated Informatics Software Approach During Method Development Using Empower 2, NuGenesis SDMS, and SDMS Vision Publisher

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Abstract

This application note demonstrates an integrated approach to capturing and storing separation related reports during chromatography method development by using Empower 2, NuGenesis SDMS, and SDMS Vision Publisher. NuGenesis SDMS acts as a data repository for analytical raw data as well as printed reports. Whereas SDMS Vision Publisher provides a reporting and authoring module incorporated as standard into NuGenesis SDMS. In addition to capturing the Empower 2 separation reports within NuGenesis SDMS, the relevant findings are composed into a summary report by using SDMS Vision Publisher.

Benefits

Reduction in associated costs, time, and effort

Introduction

Traditional chromatography method development evaluates numerous chromatographic variables that may include selection of the column, solvent, flow rate, etc.¹ Conducting a method development project often takes weeks-to-months and generates numerous chromatogram reports demonstrating the evaluation of each chromatographic condition. Organizing and maintaining the chromatographic reports for archiving purposes as well as documenting the results and writing the final method report presents an overwhelming administrative challenge to the scientist and consumes 20-40% of valuable research time that could have been applied to new projects.²

A Scientific Data Management System (SDMS) provides the ability to automatically organize and store scientific data from diverse chromatography systems as well as organize research documents. The benefits of this approach are three-fold: (1) it frees the chromatographer to focus on science while the informatics system takes care of the mundane data management, (2) electronic search tools make locating data easy, and (3) the data and results become accessible to multidisciplinary teams due to the simple user interface and global accessibility.

This application note demonstrates an integrated approach to capturing and storing separation related reports during chromatography method development by using Empower 2, NuGenesis SDMS, and SDMS Vision Publisher. NuGenesis SDMS acts as a data repository for analytical raw data as well as printed reports. Whereas SDMS Vision Publisher provides a reporting and authoring module incorporated as standard into NuGenesis SDMS. In addition to capturing the Empower 2 separation reports within

NuGenesis SDMS, the relevant findings are composed into a summary report by using SDMS Vision Publisher. Figure 1 illustrates the workflow followed in this discussion and the chromatography method was developed for simvastatin.^{3,4}

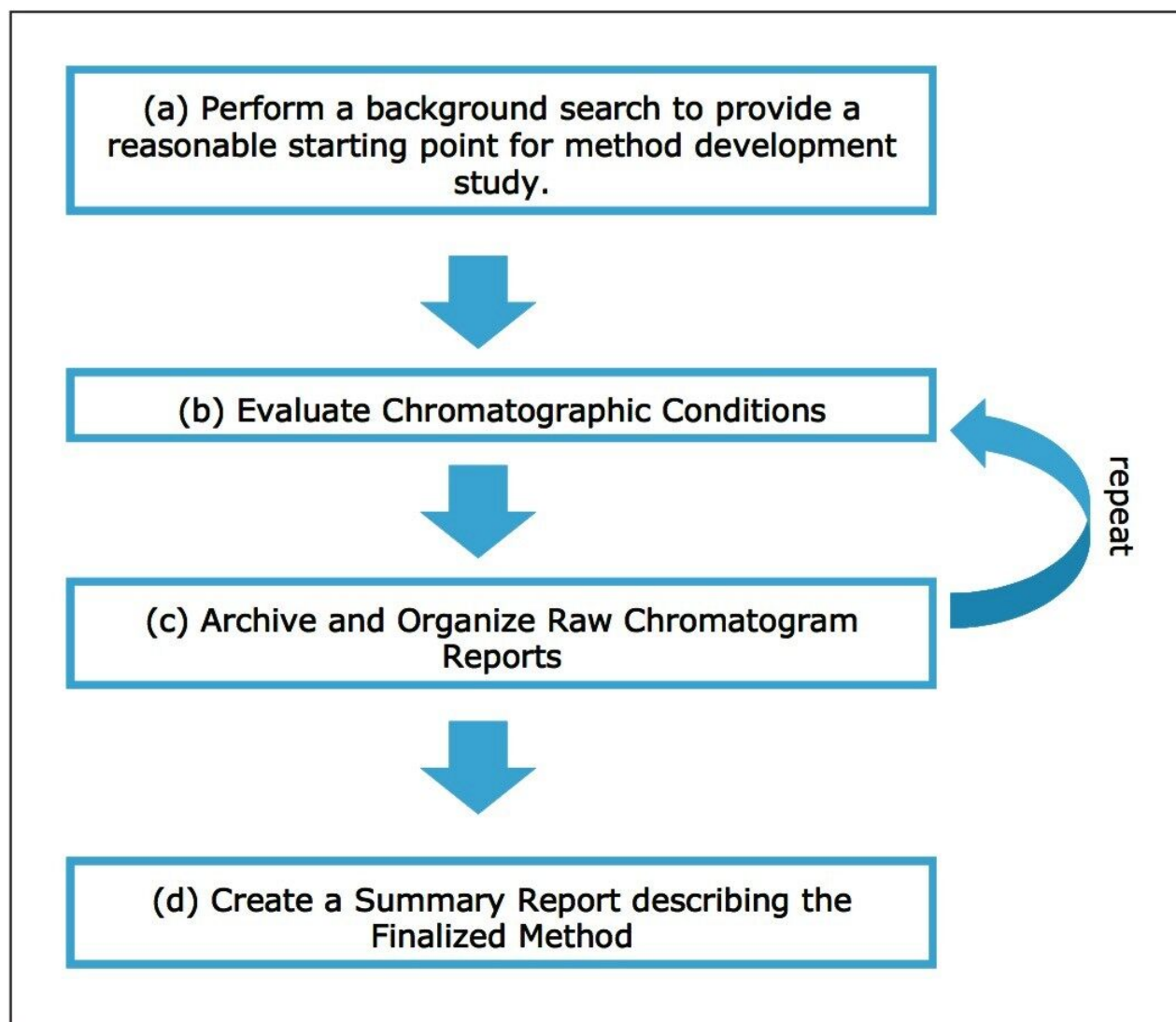


Figure 1. Method development workflow followed while employing NuGenesis SDMS to manage the chromatography reports and results.

Results and Discussion

Searching

Performing a literature search provides a logical starting point when beginning a method development project. Searching an organization's private knowledge repository for all prior research on a focus compound may return information on previously developed analytical assays, compound stability information, etc. Figure 2 illustrates an electronic search for prior research conducted on simvastatin (a cholesterol lowering compound) by using the search tool provided by SDMS Vision Publisher.

The search results produced several documents relating to previous separation studies and indicated that simvastatin degrades at pH > 6.5. Therefore, exploring pH conditions above 6.5 was an unreasonable approach. Hence, searching a globally accessible repository provided a good starting point for the proposed study.

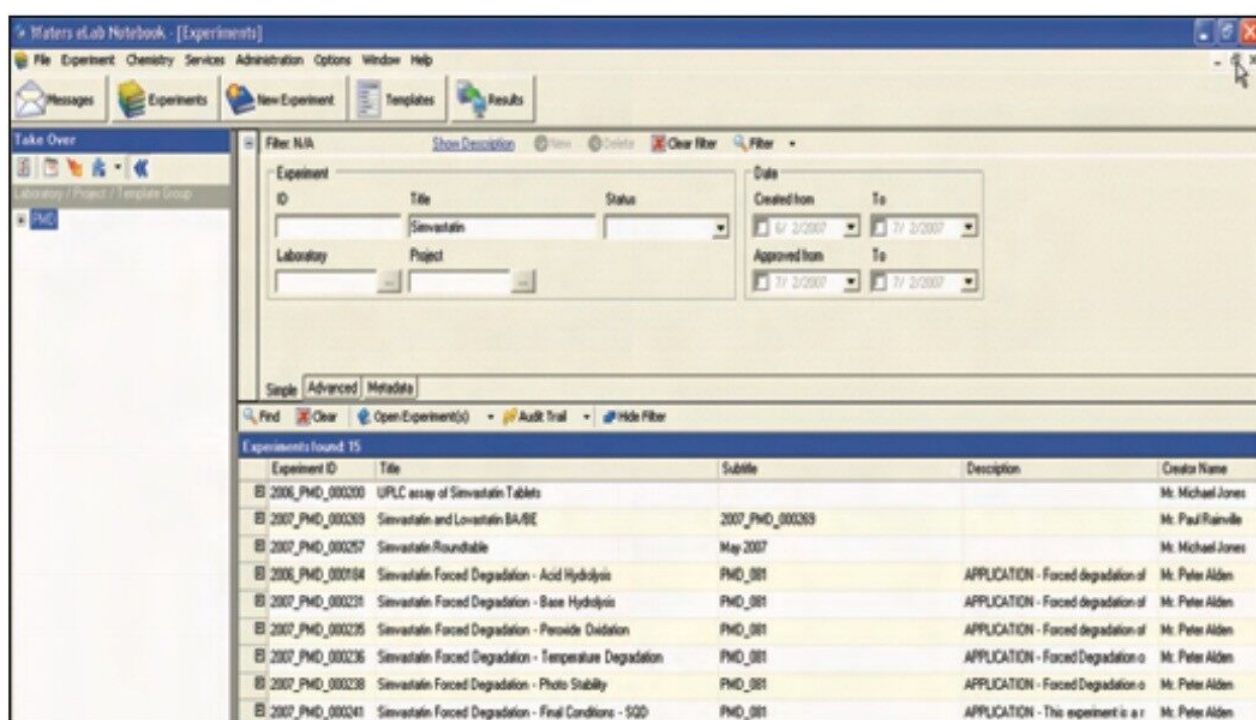


Figure 2. A search performed on the keyword "simvastatin" within Vision Publisher returns previously performed intra-company research reports.

Report Management Scenario

Chromatographers evaluate numerous chromatographic condition variables during a typical method development study and Chromatography Data Systems (CDS) manage the resulting data by either utilizing a relational database (e.g., Empower) or by storing files on a file server. However, the data and results are generally only accessible to separation specialists trained to use that particular CDS. In some cases chromatographers need to share unpolished results before writing the formal method report. For example, a NMR spectrometrists may need access to raw chromatograms while helping elucidate the structure of co-

eluting chromatographic peaks. In such cases, publishing raw separation reports into a CDS independent data repository aids in sharing results and promotes collaboration.

Figure 3 illustrates raw chromatogram reports flowing from a CDS and into a globally accessible data repository. In this case, printing Empower 2 chromatogram reports into NuGenesis SDMS after evaluating each chromatographic variable provides an easy mechanism to organize the study results. NuGenesis SDMS automatically organizes printed Empower 2 reports based on scientifically relevant text found within each report, e.g., the column type, buffer, pH, etc. Hence, locating and highlighting important findings from the chromatogram reports while writing the final method report in SDMS Vision Publisher becomes simplistic due to the streamlined data storage.

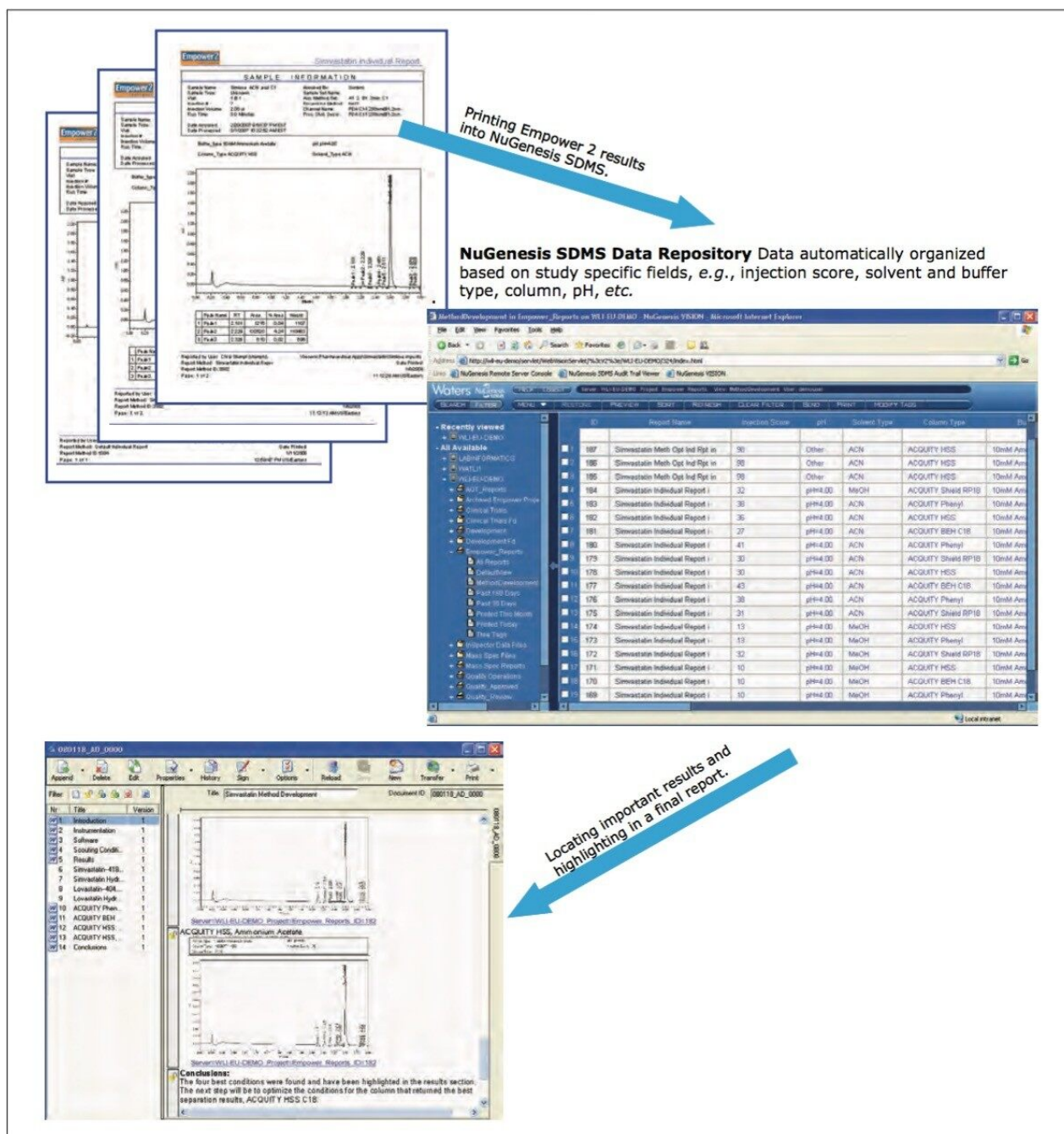


Figure 3. Empower reports are printed into NuGenesis SDMS. Then a specific subset of results is highlighted within the SDMS Vision Publisher final method report.

Figure 4 shows the final method report including chromatograms extracted from the raw Empower 2 reports stored within NuGenesis SDMS. The structured organization of the reports within NuGenesis SDMS made finding relevant information to highlight in the final report straightforward (Figure 3).

The reports were organized into columns and rows based on scientifically relevant text (e.g., project,

buffer, solvent, column selection, analyst, etc.). Sorting these descriptive columns provided an easy mechanism to evaluate one condition at a time. A particularly useful example involved a qualitative mathematical function (injection score) evaluated within Empower 2 and used to classify the quality of each chromatogram separation.

The injection score column ranked the separations from best-to- worst. See the NuGenesis SDMS Data Repository in Figure 3.

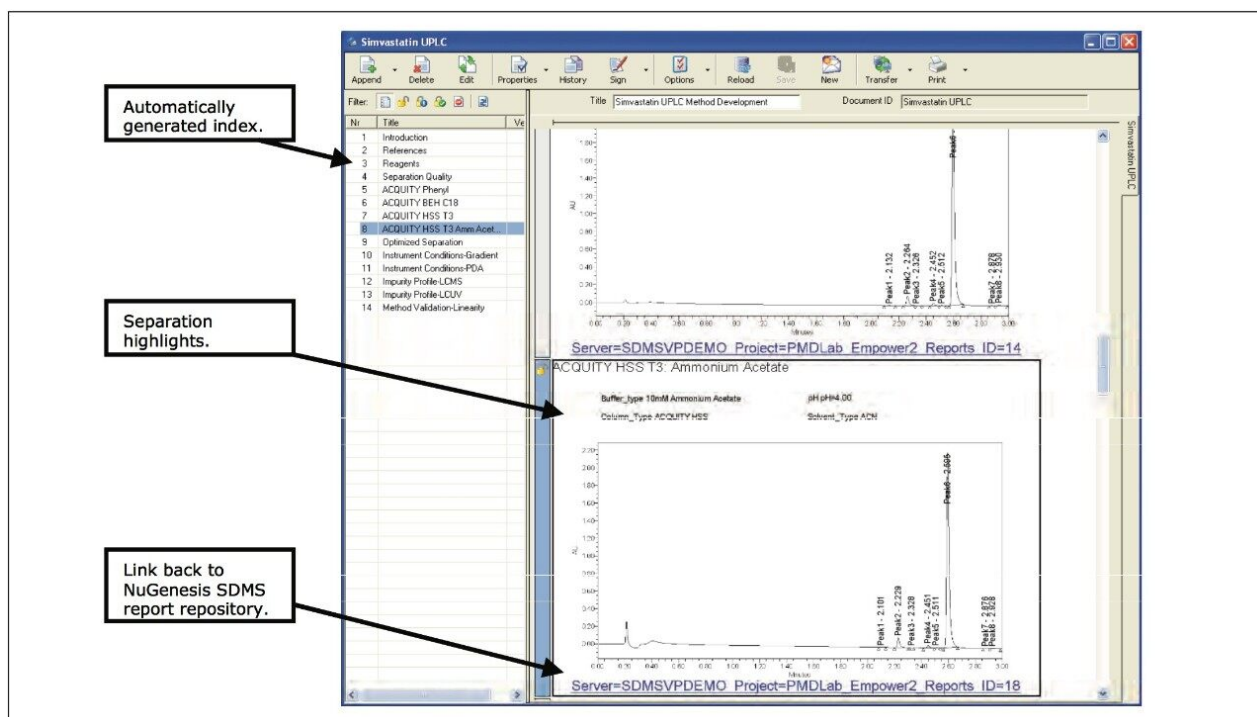


Figure 4. The SDMS Vision Publisher document describing the simvastatin method development. The chromatograms from representative separations are shown along with the links back to the original completed chromatographic reports.

Creating the Final Method Report

Hence, evaluating the overall quality of the separations became streamlined and locating representative separations for highlighting in the final report was simplified.

The final report consisted of an automatically generated index, with direct links back to the complete Empower 2 reports that have been automatically captured and cataloged within NuGenesis SDMS, an electronic audit trail that tracked edits, and an electronic signoff. Hence, documentation and data management efficiency were enhanced by about 20%. Considering published studies indicate that scientists spend 20–40% of their research time on average maintaining research data and documentation,

^{2,5} the outlined process in this application note highlights practical tools and procedures that have a direct impact on workflow and productivity.

Conclusion

Conducting an intra-company electronic search on prior simvastatin research by using the SDMS Vision Publisher embedded tools provided a reasonable starting point for the chromatography method development study thus saving valuable time and effort.

NuGenesis SDMS automatically stores, organizes, and ranks separation quality of the Empower 2 reports upon evaluating each chromatographic condition. This reduced the data management burden on the chromatographer and improved productivity by about 20%.

By publishing the reports into NuGenesis SDMS, they became globally available within the organization thus promoting multidisciplinary collaboration.

Composing a final method report within SDMS Vision Publisher highlighted the optimal separation conditions, including links back to the original raw chromatogram reports and the electronic record meets the requirements for electronic records worldwide.

Finally, with the Waters Informatics integrated solution, the often tedious and inefficient Method Development workflow can be significantly streamlined, resulting in a reduction in associated costs, time, and effort.

References

1. V G Dongre, *et al. J Pharm Biomed Anal.* 46: 236–242, 2008.
2. Electronic Laboratory Notebooks-A Foundation for Scientific Knowledge Management, Edition II. Atrium Research & Consulting: 2005.
3. European Pharmacopoeia. Council of Europe, Strasbourg Cedex. 4th Edition, 2002.
4. United States Pharmacopoeia. USP30-NF25, Page 3179, 2002. *Pharmacopoeia Forum*: Vol. 32(1) 141.
5. Ping Du, *et al. J Assoc Lab Autom.* 12(3): 157–165, 2007.

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NuGenesis ELN <<https://www.waters.com/10067209>>

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