A Self-Monitoring Quality Management System Incorporating Spectral and Chromatographic Data

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Overview

LIMS are useful in managing certain types of data for quality management and sample tracking. However, these systems are generally limited in the types of information they can process and store.

A unique automated quality management system has been developed and implemented at a fragrance manufacturer to evaluate chromatographic and spectral data of samples during quality testing. Incorporating not only conventional capabilities of sample tracking and LIMS, the new system links the live analytical data to discrete samples in a single database.

The system also carries out comparison and logic testing to further automate the process using software algorithms to make critical decisions about the quality of each sample.

The quality management system has been independently audited, and has been shown to result in a measurable increase in the effectiveness and efficiency of the manufacturing operation. This poster will outline some of the challenges in designing and implementing a system to satisfy the high throughput needs of the operation with minimal manual attendance, and how those challenges were overcome.

Introduction

The customer needed a quality assurance system that encompassed all aspects of the manufacturing process, from cataloging ingredients to quality testing finished products before shipping. The result was the development of a fully automated quality assurance system that interacts with customer's existing ERP systems to log and track samples, assess quality, make decisions, and generate reports.

Description

The solution designed to meet these needs has been described as a "spectral LIMS," differing from conventional LIMS in that the system has the ability to store, display, and search analytical spectra, chromatograms, and chemical structures as well as the full range of chemical and analytical results and metadata. The ability to handle spectra and chromatograms was essential as typical QA workflows involve comparing chromatograms and UV-IR spectra of samples with reference standards to determine whether the appropriate components are present.

The system completely automates the collection of data acquired using FTIR and GC instrumentation in real-time, executes the appropriate verification and review steps, then generates and records a pass/fail result. The automated solution is based on specific workflows that were manually carried out in the past but were time-consuming and prone to human error. Scripting and automation components, in addition to the intelligent algorithms, were employed in the system design.

Figure 1. Part of the workflow for finished fragrance products.

How it Works

A spectral database of reference materials was created, relating the chromatography, FTIR, RI, SG, and density data where available to a single product record. In this way, experimental data from all techniques could be compared as quality checks of the sample.

Expert analytical processing software provided the capability to overlay the reference spectra with the experimental spectra and to automatically analyze for similarities and differences. Any routine processing steps required for the experimental data are executed automatically by macros, ensuring uniform treatment of data.

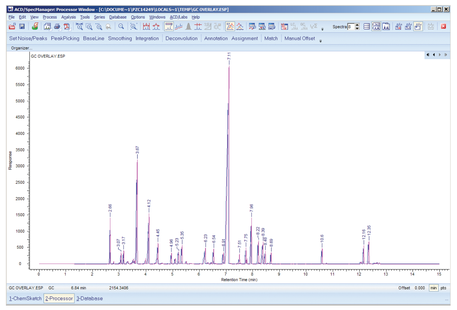

Figure 2. Spectrum overlay for sample and reference.

Various automation components, including a workflow management tool and a software controller, drive the system, triggering the execution of sample submission, processing, and interpretation steps as well as changing the status of samples and sending alerts at the appropriate times.

Flexibility in the software allowed customized forms to be developed for use in steps that require input into the system. Customized reports and an interface to view and search the system were also implemented.

Sample submission within the company's ERP system, which ties customer orders with quality control and eventually shipping, triggers a request in the QA system. FTIR and RI/SG/density are measured and data is automatically swept from the various instruments into the system in real time. Processing, analysis, and interpretation steps are then executed on each sample file.

Alerts are triggered during steps that either require manual intervention (i.e., review check by a perfumer) or when a sample fails a check.

Upon completion of the process, all information pertaining to each sample is stored fully in the database and, if appropriate, a certificate of analysis is produced. Successful samples are released to the ERP system, which then proceeds to order fulfillment.

Challenges

Several challenges had to be overcome in the course of developing the QA system. Some were resolved simply through the capabilities of the software and automation components, and others required innovative solutions.

Developing a searchable spectral and chromatographic database was central to the project, as the QA workflow involves comparing experimental and reference spectra for an acceptable match. Uniform processing of data was also critical to ensure that comparisons could be made. This is especially true of chromatographic data, which tends to have greater variability depending on instrumentation, methods, and parameters. Existing software was able to do this with algorithms for the appropriate processing. ACD/Labs software is capable of importing data files from most major instrument vendors so that the use of different instrumentation was not an issue.

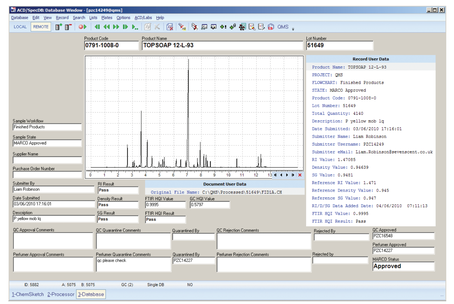

Figure 3. Example of a screen form.

The system had to conform to the rigid workflows already in use by the customer. The workflow includes not only analytical data handling steps but also review checks done automatically and by professional perfumers. The challenge of routing samples appropriately was overcome with the use of scripting to complement out-of-the-box workflow management software.

Finally, the system had to integrate with an existing ERP with the ability to pull information and push back useful results at the end of the process. Integration was accomplished with scripts provided by ACD/Labs Professional Services staff.

Conclusion

Despite challenges, it is possible to use software to create a fully automated QA system using commercially available software and a small amount of customization. The benefits realized with the automated system are markedly improved quality standards, increased productivity, and throughput requiring minimal user attendance.

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