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Case Study - P1

Purification Laboratory Workflow and Sample Tracking

Business Case

A major pharmaceutical company wanted to increase throughput dramatically in their purification lab. They identified a suitable piece of equipment for the task, in this case a Waters purification factory (fig. 1). The machine uses a mass spectrometer to identify peaks of interest and diverts fractions into glass vials. The factory has a unique feature in that it will inject and analyse 4 samples simultaneously using a liquid multiplexer, and is coupled to 4 fraction collectors. This allows a much higher throughput than traditional single injection systems.

Fig 1. The Waters purification factory

The client realised that the staff workload would increase in managing all the other processes before and after the purification step. Samples had to be registered when they arrived in the lab and a pre-analysis was desirable to reduce the number of samples presented to the factory for purification. Each purification run of four 48 well plates could generate up to 1,152 glass vials, each of which would then be evaporated, re-dissolved to a known concentration and the best fractions pooled into a final vial for registration.

It was clear that all the plates and vials would need to be tracked through the lab. A sample could be in the lab for a few days resulting in thousands of vials in racks at different stages of the process. In addition status information needed to be presented to the users so that decisions could be made about each sample.

Designing the solution

Prior to the installation of the purification factory, Aitken Scientific worked closely with the client and Waters personnel to define the precise process to be implemented in the lab. Important decisions were made such as the need to use bar-coded vials at all stages, with the barcode etched into the glass. Each rack of vials would also be bar-coded so that collections of vials could be moved around the lab and identified together.

Each step in the process was looked at in some detail from the ergonomic point of view. How would the lab chemists actually perform the step. Where should the barcode readers be, and how many PCs would be needed for the work to progress smoothly. Aitken Scientific also assessed the selected hardware, such as the Zinsser Analytic Calli liquid handler (fig 2), to see if they could be automated. It would be more efficient if the software could tell the liquid handler what liquid movements were to be done allowing the operator to place vials for dissolution or pooling in any location in a rack.

Fig 2.
The Zinsser Analytic Calli liquid handler.

Finally, Aitken Scientific designed a simple sample tracking solution which would allow easy operation by the users. This was prototyped before implementation began to ensure suitability in the lab environment. The solution reduced the workload considerably, and also reduced the potential for errors.

The Sample Tracking Software

Some of the data needed by the sample registration process was stored in the client's existing Oracle® databases. Therefore, the solution was designed around a new Oracle® database located on a server within the client's IT environment. Sample plates had identifiers which would allow data for individual wells to be extracted and copied into the sample tracking database.

The solution allows any plate, vial or rack in the system to be scanned and the related original plate identified. So at each stage, plates, vials and racks of vials are traceable back to an original sample plate. For example, when vials are removed from a rack and placed into an evaporator, the association between the vial and original sample plate is maintained. When a vial or rack is finished with, the relationship to the original plate is removed, allowing the vial or rack to be re-used. Using the relational database made this task straightforward.

The original plate is considered the master reference. The software tracks all the processes that the plate has been through. This is represented graphically using icons joined together by arrows (fig 3). Any icon can be selected to show what had happened at that stage.

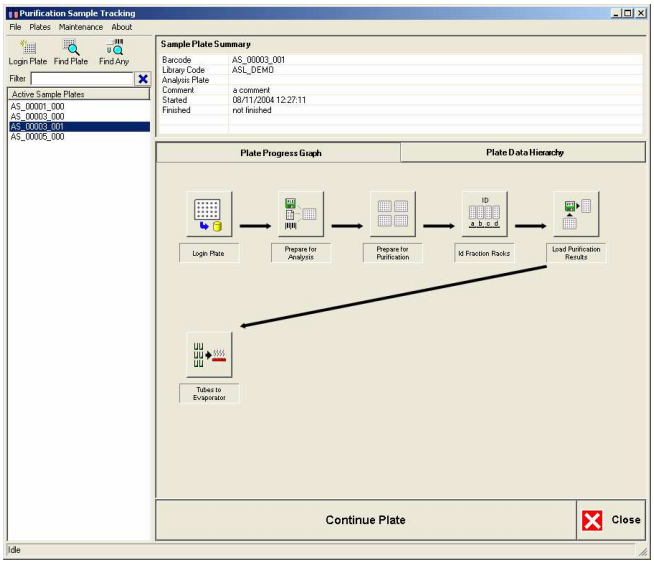

Fig 3. Showing the processes related to a sample plate.

The Stages

Each stage in the process was written as a single software component which plugged into a core application. The core needed to know nothing about the detail of the processes that it supported. All it needed to know was that samples had arrived and had been processed by the individual stages. Each component had the same interface functions and drew its own dialogue on the right hand side of the main screen. (fig 4).

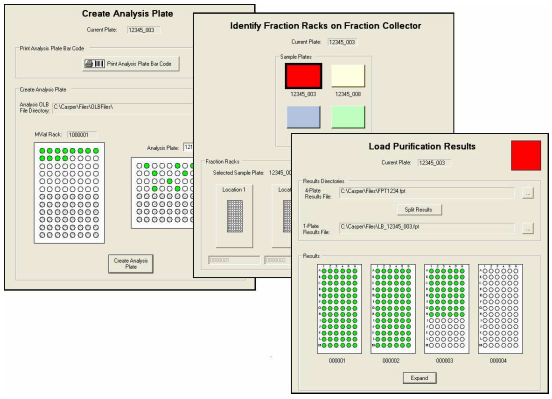

Fig 4. Examples of the individual component dialogues

The overall flow of processes was defined by an XML file. This listed the names of each stage, the name of the component program which contained the implementation of the stage, and the names of the stages which the user could do next. In this way the workflow could be rearranged without programming.

Reports

The data contained within the Waters data files included complete chromatograms and mass spectra. To allow the chemists to evaluate the process, they needed to see the pre-analysis, purification and post-analysis data at the same time. Aitken Scientific developed a viewer which provides the client with access to all the data at the same time, including data held in the Oracle® database, allowing them to mark samples for further processing.

Benefits

Within a few months, the lab was handling more than the target throughput. The client realised that by moving to a double shift pattern even more samples could be handled, saving the company the cost of outsourcing this important process. Aitken Scientific was retained to provide an enhancement to the software to support 8 plates being placed on the mass spec at a time, instead of the original 4.