{ APPLICATION NOTE }

Implementing sample management software for the first time - Mosaic SampleBank™

Mark Doring. Titian Software Ltd

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Mosaic Sample Management is Titian Software's comprehensive, customisable, modular software product to control and monitor all aspects of sample storage, preparation and delivery. From small biotech to global pharma, Mosaic helps to provide a seamless, error-free sample supply chain and audit trail. Mosaic Sample Management is a tailored solution for all sample management requirements, configured through expert consulting services.

Mosaic SampleBank™ and Mosaic FreezerManagement are Mosaic packages, optimised and pre-configured for rapid deployment:

- FreezerManagement keeps track of samples in freezers and provides a comprehensive audit trail as samples are accessed and aliquoted.
- SampleBank provides full inventory tracking capabilities coupled with sample ordering and workflow management in a simple package. It offers seamless start-up and ongoing performance for busy sample managers.

Mosaic's modular approach means that it is simple to upgrade or extend the software's functionality whenever it is needed.

Introduction

The tracking and management of samples is becoming ever more important in research and development organisations. These samples may represent highly valuable assets, the tracking of which cannot just be trusted to a spreadsheet. In some cases, sample management, screening and automation may be performed by just one person, who is under significant pressure to provide:

- Accurate inventory information
- Rapid fulfilment of sample requests
- A high quality audit trail of how the samples are changed

To achieve this cost-effectively for a growing company requires a robust tool for sample oversight and workflow management to enable the effective storage, retrieval and processing of samples while making the most efficient use of supporting automated instrumentation. Titian's Mosaic SampleBank™ software has been developed with these essential needs in mind.

Titian Software has listed closely to the feedback of its customers over the years and has developed SampleBank to be a lightweight, pre-configured version of Mosaic that can be deployed quickly, while still providing the robust sample management solution that the industry has grown to depend on.

SampleBank features include:

Ordering and workflow fulfilment

- Create and manage sample processing requests and fulfilment workflows (e.g. weighing, dispensing, storage)

Intuitive web-based user interfaces

- Manage samples, depict the layouts of stores accurately, pick and place to stores with ease
- Simple deployment to requestors

Audit trail

- Capture every action in a comprehensive audit trail; an essential requirement for regulated environments, or for report generation using precise metrics

Bulk upload facility

- Tubes and substances may need to be created, edited or discarded in bulk (e.g. disposal of materials past expiry). It may also be necessary to import data from a legacy system, or receive bulk shipments from outside sources, such as CRO's and compound providers. File import mechanisms with robust error checking are provided for this.

Searching

- Easily find samples based on any of the available sample and container parameters using flexible inventory search tools

Expandability

- SampleBank offers a pre-configured environment with the flexibility to expand as your needs grow. Additional features and expanded Mosaic functionality can be unlocked as appropriate.

SampleBank Customer Analysis – A Key Phase in Implementation

Important questions for sample managers to ask before selecting a solution

Expectations:

- What is the scope of the sample management effort?
- What goals does the company want to achieve with a sample management system?
- What processes can be improved upon?

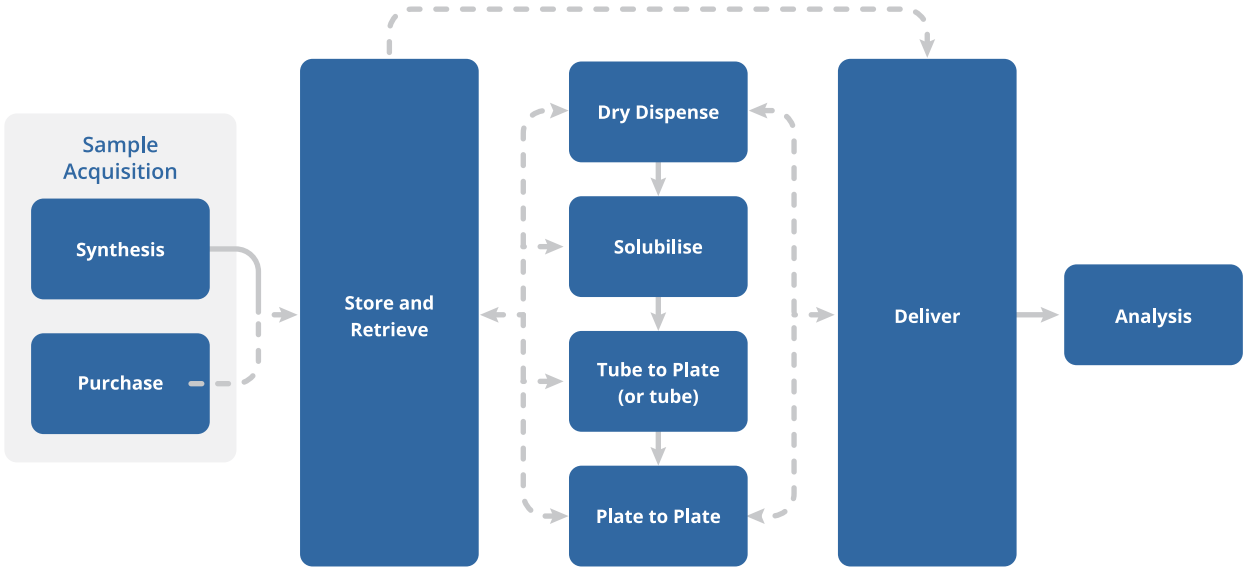
Things to consider:

- Workflow and current processes
- Bottlenecks and/or obstacles to productivity
- Automation/capital equipment to be integrated
- IT infrastructure and support
- Connectivity with other departments
- Standardisation of labware and output formats (plate maps, etc.)
- Users and what their roles should be
- Rules and restrictions around sample access
- Future expansion capabilities

Analysing Business Processes

The areas to assess before choosing dedicated sample management software can be illustrated by working through a generic sample management workflow for a small company (see Figure 1). This initial assessment will ensure the benefits of the solution are fully realised on implementation.

Figure 1: Simplified SampleBank workflow



The Sample Management Workflow

Sample acquisition

- Synthesis of biological and/or chemical samples by company sources
- Purchase of samples from CROs, compound library providers, etc.
- Registration of materials in electronic lab notebooks (ELNs)
  - To accommodate multiple substance types, SampleBank includes its own internal substance registration system, and can easily be configured to integrate with one or more external ELN or substance registration systems.

SampleBank workflow management

- Storage and retrieval of samples
  - Inventory control for request management and fulfillment
  - Pick and place operations to stand-alone and/or automated† stores
- Dry dispensing†
  - Weighing of samples for delivery, storage or downstream solubilisation
- Solubilisation
  - Dissolution of samples to desired concentrations
- Liquid handling† to fulfill orders in accordance with the sample requests
  - Tube to plate (or tube) transfers
    - Single point/concentration transfers, serial dilutions, creation of aliquots, etc.
  - Plate to plate transfers
    - Multichannel pipetting operations (e.g. plate stamping, quadrant transfers, serial dilutions, single channel cherry picking)
- Deliver
  - Automatic fulfillment completion notifications through email

Data analysis

- Downstream evaluation of prepared samples in biological and/or chemical tests
  - e.g. Integration with assay data analysis systems

†For supported Mosaic integration solutions, see Titian's Mosaic Integration Brochure.

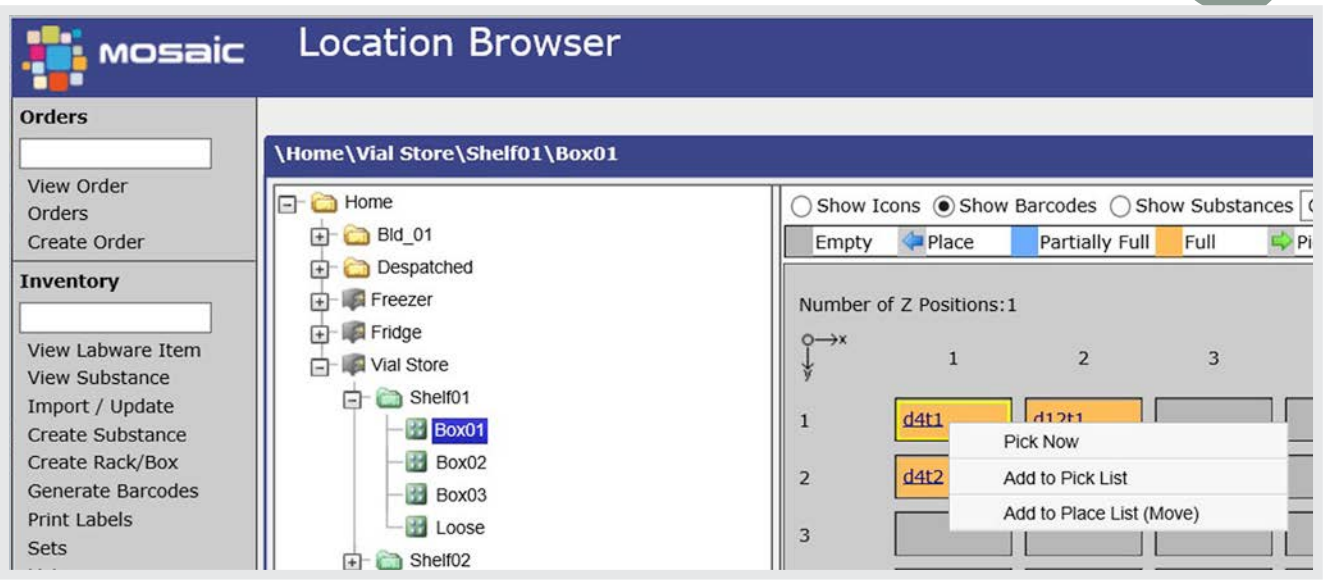
SampleBank Components

Sample inventory storage

The way in which samples are stored varies from company to company. Storage methods can take the shape of one (or more) large automated store(s), multiple smaller automated stores, cold rooms, freezers, cryogenic containers, desiccators or some combination of all of the above to meet the disparate needs of the samples being stored. The stores can also be physically co-located in the same lab, or exist in different labs or building locations depending on a variety of factors and company preference. Whatever the case, you can configure these locations in Mosaic SampleBank to make it easy to know the exact whereabouts of your valuable samples at any given time.

The fast and accurate location of samples means no time is lost searching for them. The easy recording of sample picking ensures that inventory records are kept accurate.

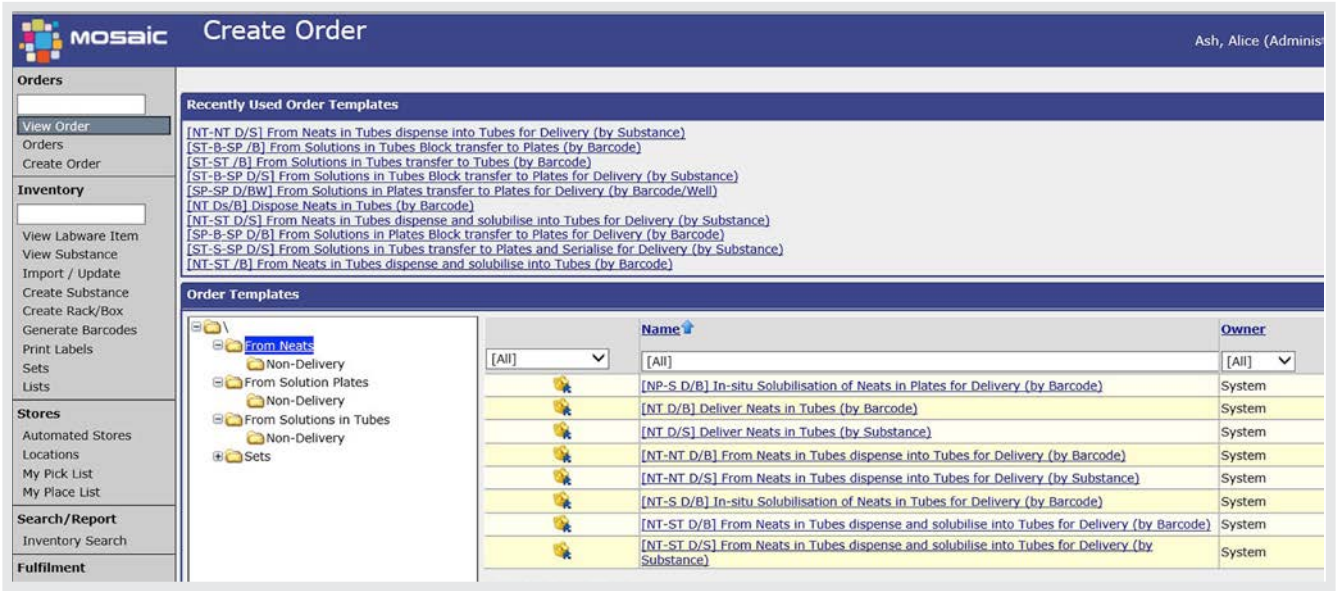
Figure 2: Location browser



Ordering

Mosaic SampleBank's order templates covering basic sample management processes are already pre-configured for your use. These basic operations have been tested comprehensively, and cover the most common processes used by our customers (e.g. the dispensing of dry powders, creation of stock tubes, serialised plates for delivery, etc.).

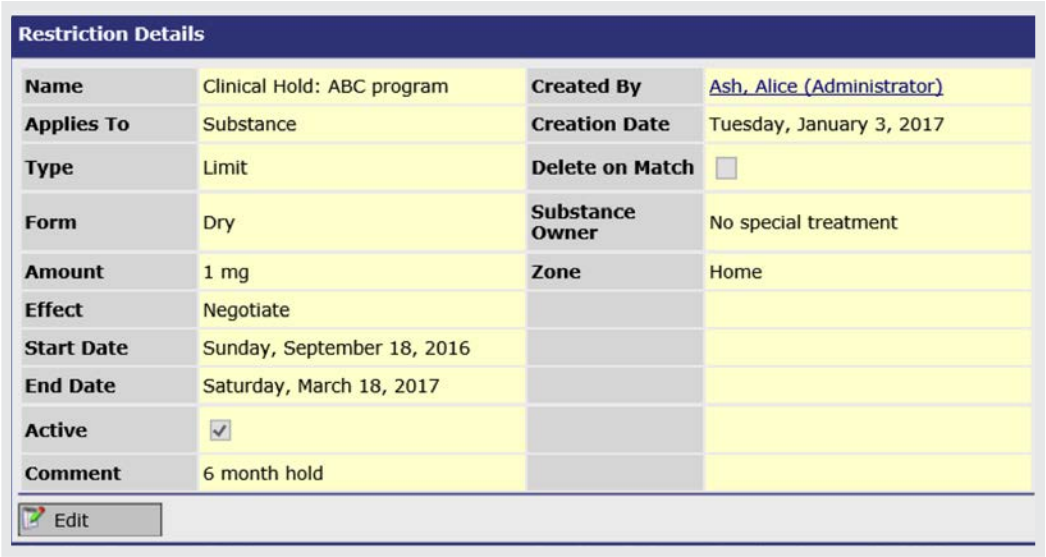
Figure 3: Order creation



Substance restrictions

Substances and/or labware can have restrictions placed on them to limit their availability for ordering. Users define the criterion for the restriction through a simple GUI, as well as how to react to a request for the item(s) assigned to the restriction.

Figure 4: Substance restriction example



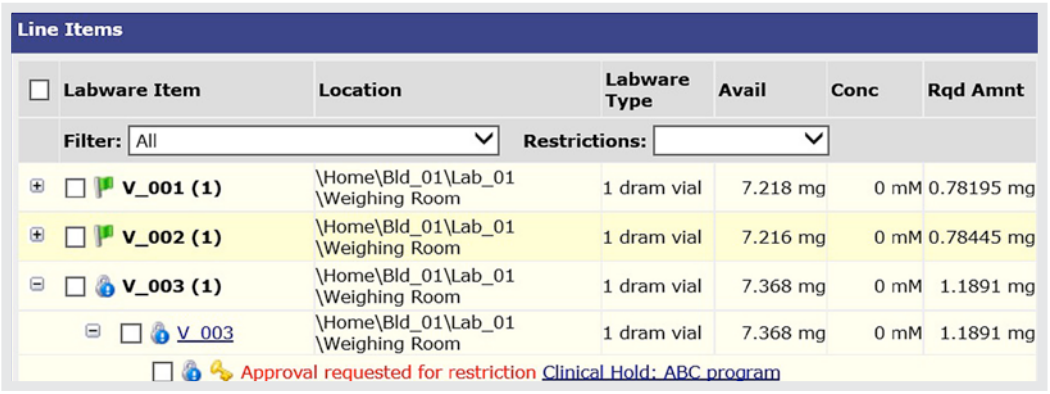
Restriction Details

Name	Clinical Hold: ABC program	**Created By**	Ash, Alice (Administrator)
Applies To	Substance	**Creation Date**	Tuesday, January 3, 2017
Type	Limit	**Delete on Match**	☐
Form	Dry	**Substance Owner**	No special treatment
Amount	1 mg	**Zone**	Home
Effect	Negotiate		
Start Date	Sunday, September 18, 2016		
End Date	Saturday, March 18, 2017		
Active	☑		
Comment	6 month hold		

Edit

In the example above, if more than 1mg of the substance is requested in an order during the restriction period, an email will be sent to the substance owner to approve or deny the request.

Figure 5: Line items view of restricted sample



Line Items

Labware Item	Location	Labware Type	Avail	Conc	Rqd Amnt
Filter: All		Restrictions:			
V_001 (1)	\Home\Bld_01\Lab_01 \Weighing Room	1 dram vial	7.218 mg	0 mM	0.78195 mg
V_002 (1)	\Home\Bld_01\Lab_01 \Weighing Room	1 dram vial	7.216 mg	0 mM	0.78445 mg
V_003 (1)	\Home\Bld_01\Lab_01 \Weighing Room	1 dram vial	7.368 mg	0 mM	1.1891 mg
V_003	\Home\Bld_01\Lab_01 \Weighing Room	1 dram vial	7.368 mg	0 mM	1.1891 mg
Approval requested for restriction Clinical Hold: ABC program					

When populating line items in an order, a restriction will show up allowing the compound manager to see that an approval is pending for the restricted material.

Independent of restrictions, the amount required by the order is also reserved, so that other requests cannot affect the completion of this Order.

Workflow management

When a Mosaic SampleBank order is created and submitted for fulfilment, a validated Mosaic workflow is generated which defines all the steps needed to create the outputs specified in the order. In the example below, an order has been placed to create three substance solutions from dry stock at a concentration selected by the Requestor. The Requestor also selects a desired volume, and includes an acceptable volume range to allow the compound manager some flexibility in weighing out the required molar quantity. The samples will be weighed in accordance with these parameters, solubilised, and then delivered to a specified location for Requestor pickup.

Figure 6: Order workflow example

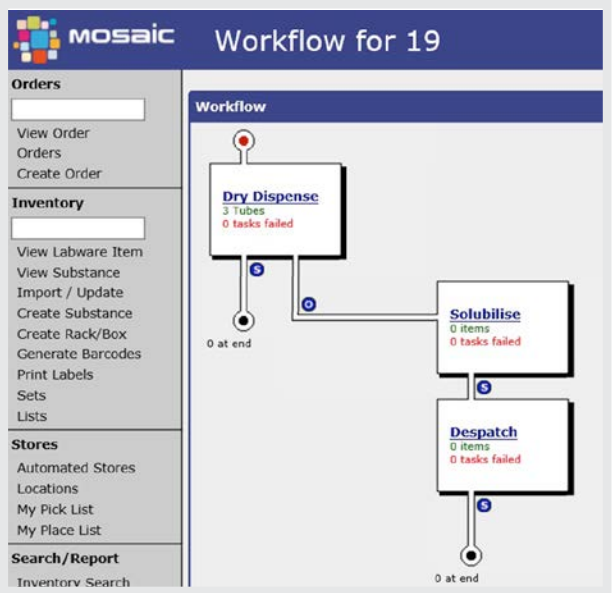
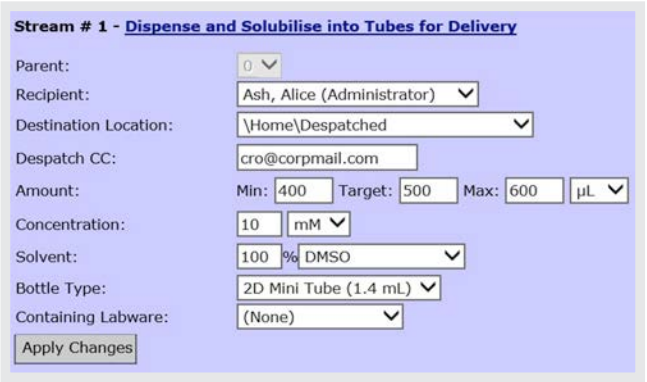


Figure 7: Selection of output parameters



Distribution of samples

Keeping on top of who has requested which sample can be a logistical challenge without software to manage requests and their delivery. The dissemination of order parameters (e.g. order summary information, serialisation schemes, plate maps, etc.) can also be a time-consuming endeavour for compound managers. SampleBank facilitates this process for you with accurate and timely delivery information.

Sample Despatch Note

This despatch contains items for the following order:

# Line Items in Order	3
Order Template	[NT-ST D/B] From Neats in Tubes dispense and solubilise into Tubes for Delivery (by Barcode)
Order Comment	
Concentration	10 mM
Delivered	Thursday, December 29, 2016 1:54 AM
Delivery Location	\Home\Despatched
Labware Type	2D Mini Tube (1.4 mL)
Layout	
Order	19
Requestor	Ash, Alice (Administrator)
Solvent Conc	100%
Solvent	DMSO
Target Amount	250 µL

Notifying the scientist that their samples are ready for pick-up or in transit ensures samples are not overlooked. Configurable Excel files containing dispense layouts, etc. can also be attached automatically.

Automated emails also mean one less thing to do for busy SampleBank operators!

Sample tracking

Managing one (or more) barcode ranges and ensuring their ongoing uniqueness is vital for efficient operation, but almost impossible when using a spreadsheet. SampleBank keeps track of barcodes for you; whether you label your labware yourself, or use pre-barcoded labware.

ABC12345

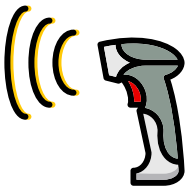
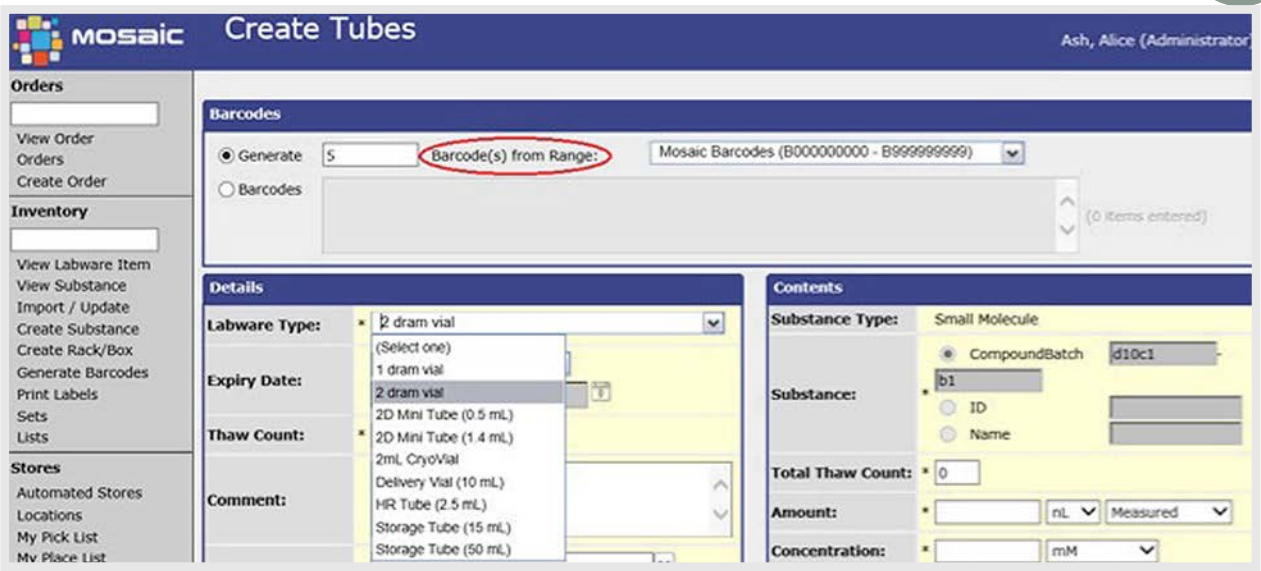


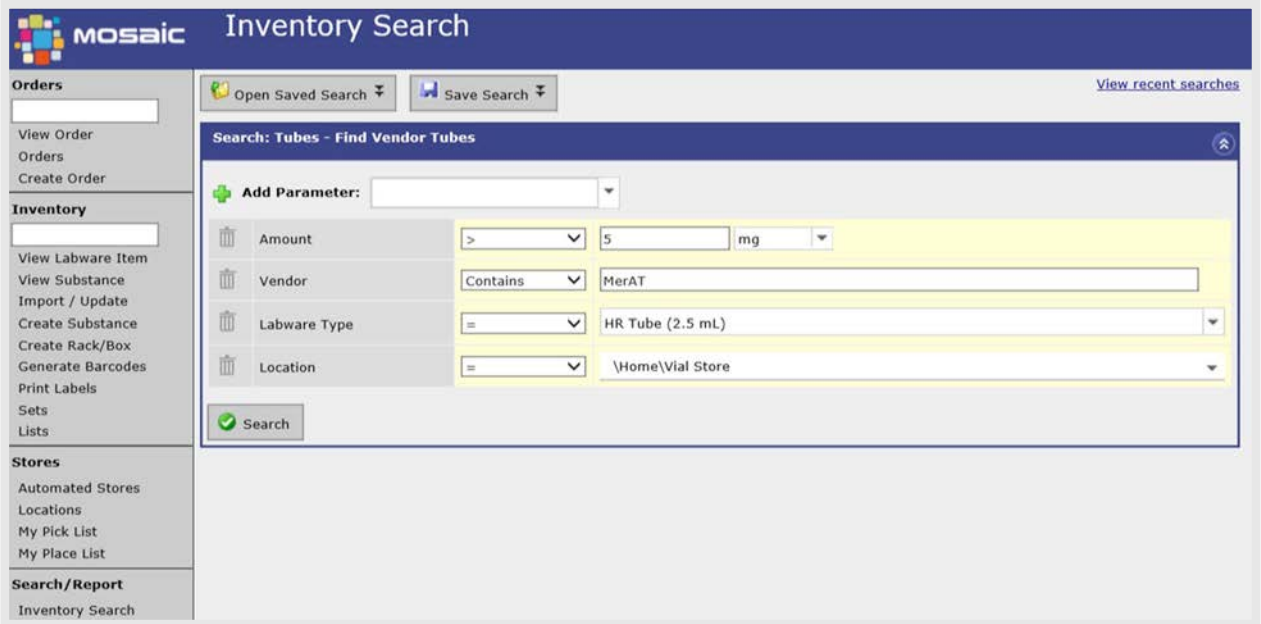
Figure 8: Creation of tubes/vials with unique barcode identifiers



Inventory search

Scientists should to be able to search inventory to find their materials of interest themselves, and not rely on back-and-forth email communications with sample managers. Dedicated search and request tools make this easy.

Figure 9: Searching the Mosaic SampleBank inventory

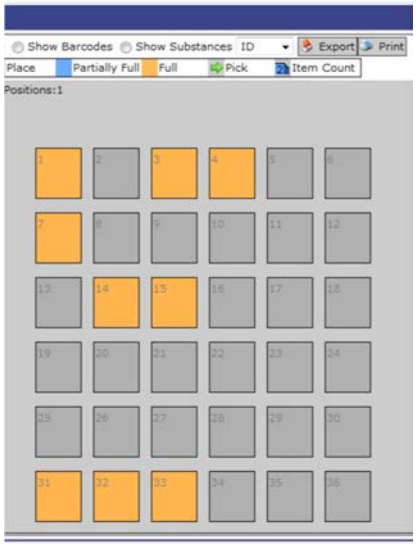


Search queries which are frequently used can be saved, and search results can be exported to Excel for inclusion in reports, etc Comparison tools are also available to combine, subtract, or find the common elements between individual search results.

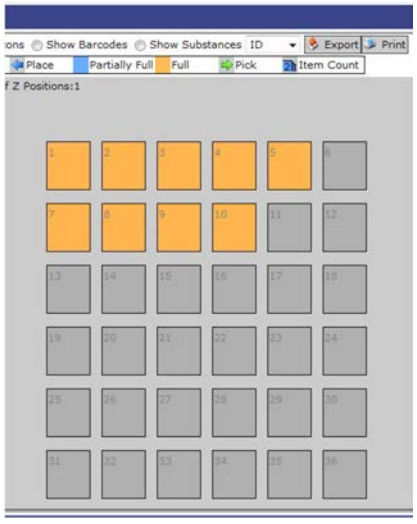
Manage Manual Inventory in 3 Easy Steps – SampleBank 2D Barcode Rack Scanner Integration

One of the most accurate and efficient ways to manage the inventory of tubes in manual freezers or cryo-storage is to use 2D-barcoding technology and a dedicated scanner for reading multiple tubes in a rack simultaneously. Mosaic's Tube Position Verifier (TPV) application provides the interface to both the inventory data and the rack scanners to provide seamless reconciliation of physical tube positions and their record in inventory. This allows you to pick, place or re-array tubes with incredible accuracy.

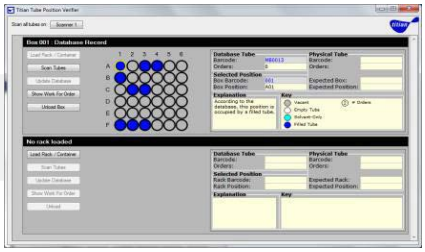
The illustration below shows how simple it is to re-array a box of 2D-barcoded tubes using Mosaic's TPV and a rack scanner.



Here 2D Rack Scanner integration can is used to rearrange 2D barcoded tubes in a freezer box. It is also used to Pick or Place items to/from stores and racks – all at the click of a button

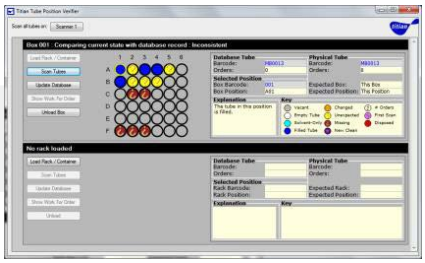


1 **Scan freezer-container using TPV application**



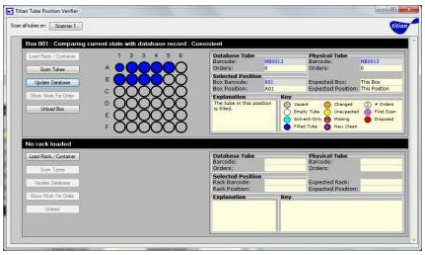
Tubes are read and displayed in their current positions

2 **Re-arrange tubes and re-scan**



Conflicts between scan and inventory record are displayed

3 **Click to update database**

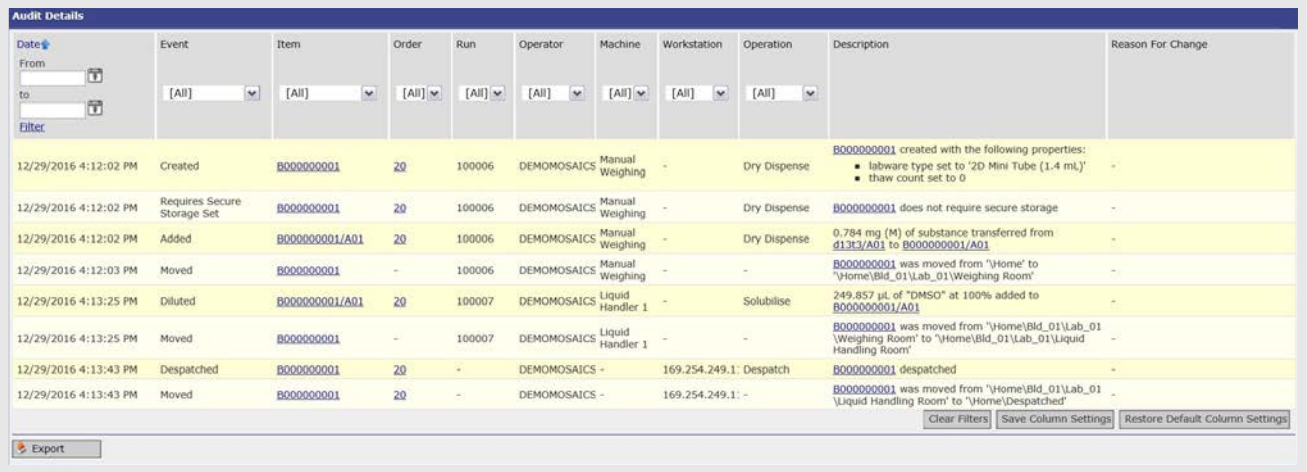


Inventory record and scan now agree

Comprehensive Audit Trail

Complete "cradle-to-grave" sample tracking is what you get with Mosaic SampleBank. At the click of a mouse, you can find out where samples are in process, and what operations have been performed on them and by whom. Results can be viewed and exported for further analysis, as needed.

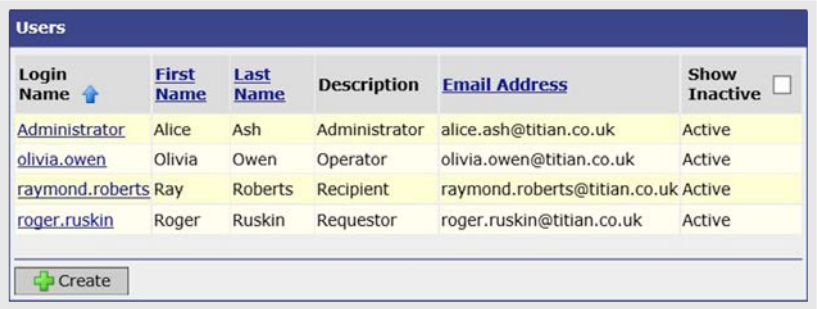
Figure 10: Audit trail example



Management of Users and SampleBank Permissions

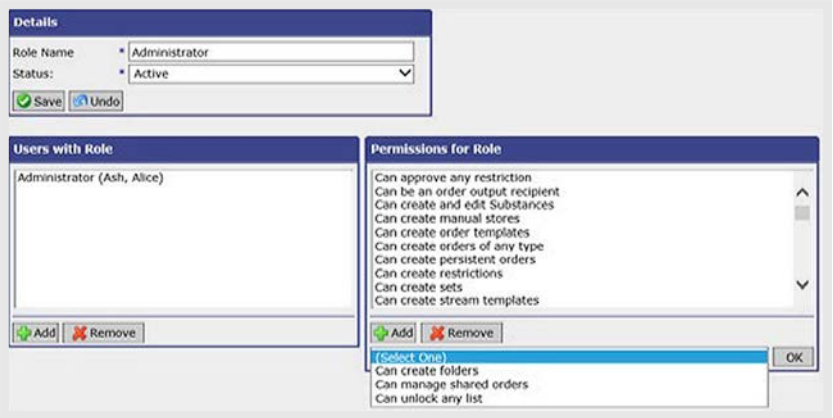
Mosaic SampleBank gives you full control over what system users can and cannot do within the software. Administrative users are able to assign and adjust permissions as needed, as well as create new users and roles based on your own corporate practices.

Figure 11: User examples



Permissions for SampleBank roles are also managed through an intuitive GUI.

Figure 12: Selection of role permissions



Automation Options Available in Mosaic SampleBank 7.0

Available integration with

- Analytical balances (e.g. Sartorius, Mettler-Toledo)
- 2D microtube rack imaging systems
- Automated sample stores (e.g. Hamilton, TTP Labtech)
- Tecan Freedom EVO liquid handlers
- Labcyte Echo/Access systems
- Microtube sorters (e.g. BioMicroLab)
- Substance registration/ELN systems (e.g. ChemAxon, etc.)
- Data analysis systems (e.g. IDBS ActivityBase, etc.)
- TTP Labtech mosquito

Run-file management is available for additional automated liquid handling systems

- (e.g. Hamilton Microlab-STAR, Agilent Bravo, Beckman Biomek etc.)

Additional Mosaic integrations are available upon request

- Mosaic 7.0 applications
  - VFM (for Agilent VWorks)
  - FHLH (for liquid handling systems with multiple pipetting heads)
  - CFM (for HighRes Biosolutions' Cellario)
  - etc

Summary

This application note illustrates many of the benefits of using Titian's Mosaic SampleBank software to get you started quickly and efficiently in sample management with a robust, industry proven solution. SampleBank's lightweight, pre-configured deployment provides the functionality to: acquire, update, store, order against, transform, and track inventory for companies with simple or diverse sample collections. The product supports almost any sample type (e.g. small molecules, antibodies, cell lines, DNA, etc.), and can be integrated with a variety of instrument types (automated stores, 2D scanners, balances, etc.) Through use of Mosaic software, Titian's customers have realised significant benefits in terms of throughput, fulfilment response times, error rate reduction, labour costs and sample conservation.

As your needs grow, the Mosaic SampleBank solution can be extended to grow with you. Adding in additional Mosaic functionality, adopting additional workflows, or integrating additional instrumentation can all be configured as your needs expand. Titian constantly looks to improve the product and provide connectivity with the latest automation technologies that support sample management methods. Workflows involving multiple activities and higher complexity can also be incorporated as these requirements emerge. Titian welcomes the opportunity to work with customers and industry partners to explore future enhancements, and to provide the best sample management solution for your current and future needs.

About the author

Mark Doring

Mark Doring worked for Schering Plough for 25 years as a biochemist in new lead discovery, focusing on high throughput screening assay performance, development and compound preparation with an emphasis on automation and informatics. He joined Titian Software in 2015 as a business application consultant.

Notes

Notes

Titian Software Ltd

2 Newhams Row,
London SE1 3UZ
UK

Tel: +44 20 7367 6869
Fax: +44 20 7367 6868

1500 West Park Drive,
Westborough MA 01581
USA

Tel: +1 508 366 2234
Fax: +1 508 366 2744

info@titian.co.uk
www.titian.co.uk