

{ APPLICATION NOTE

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

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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.

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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 colocated 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

iii Mosaic	Location Browser					
Orders View Order Orders Create Order Inventory	Home\Vial Store\Shelf01\Box01 Image: Constraint of the store of the st	Empty Number of	cons) Show Place of Z Positions	w Barcodes) Sh Partially Full :1	ow Subst	ances [(
View Labware Item View Substance Import / Update Create Substance Create Rack/Box Generate Barcodes Print Labels Sets		\downarrow 1 2 3	1 d4t1 d4t2	2 Pick Now Add to Pick List Add to Place List (M	3 tove)	

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

iii Mosaid	_ Create Order		As	h, Alice (/	Admir
Orders					
	Recently Used Order Templates				
View Order Orders Create Order Inventory View Labware Item View Substance Import / Update	INT-NT D/S1 From Neats in Tubes dispension [ST-8-5P /B] From Solutions in Tubes Bit [ST-9-5P D/S1 From Solutions in Tubes Bit [ST-9-5P D/S1 From Solutions in Index St [NT-ST D/S1 Prom Solutions in Plates tr INT Os/8] Dispose Neats in Tubes (by Ba INT-ST D/S1 From Neats in Tubes (by Ba [ST-9-8-5P D/S1 From Solutions in Plates St [NT-ST D/S1 From Neats in Tubes dispension]	ick transfer to Plates (by Barco fer to Tubes (by Barcode) lock transfer to Plates for Delivy ansfer to Plates for Delivery (b rcode) se and solubilise into Tubes for lock transfer to Plates for Deliv ansfer to Plates and Serialise f	ie) ery (by Substance) / Barcode/Well) Delivery (by Substance) ery (by Barcode) or Delivery (by Substance)		
Create Substance Create Rack/Box	Order Templates				
Generate Barcodes	BC \ BC From Neats		Name	Owner	
					~
Print Labels Sets	O Non-Delivery	[All]	[All]	[All]	
	Non-Delivery		[All] [NP-S D/B] In-situ Solubilisation of Neats in Plates for Delivery (by Barcode)	[All] System	
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ets sts ores utomated Stores ocations y Pick List	Non-Delivery Control Solution Plates Non-Delivery Control Non-Delivery Control Non-Delivery Non-Delivery		[NP-S D/B] In-situ Solubilisation of Neats in Plates for Delivery (by Barcode) [NT D/B] Deliver Neats in Tubes (by Barcode) [NT D/S] Deliver Neats in Tubes (by Substance)	System System System	
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ets ists ores utomated Stores ocations ly Pick List	Non-Delivery Control Solution Plates Non-Delivery Control Non-Delivery Control Non-Delivery Non-Delivery		[NP-S D/B] In-situ Solubilisation of Neats in Plates for Delivery (by Barcode) [NT D/B] Deliver Neats in Tubes (by Barcode) [NT D/S] Deliver Neats in Tubes (by Substance) [NT-NT D/B] From Neats in Tubes dispense into Tubes for Delivery (by Barcode) [NT-NT D/S] From Neats in Tubes dispense into Tubes for Delivery (by Substance)	System System System System System	

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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
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Name	Clinical Hold: ABC program	Created By	Ash, Alice (Administrator)
Applies To	Substance	Creation Date	Tuesday, January 3, 2017
Туре	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	V		
Comment	6 month hold		

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.

	Labware Item	Location	Labware	Avail	Conc	Rqd Amnt
_			Туре			•
	Filter: All	✓ Rest	trictions:	~		
Ð	🗌 🏴 V_001 (1)	\Home\Bld_01\Lab_01 \Weighing Room	1 dram vial	7.218 mg	0 mM	0.78195 m
Ð	□ 🏴 V_002 (1)	\Home\Bld_01\Lab_01 \Weighing Room	1 dram vial	7.216 mg	0 mM	0.78445 m
Ð	🗌 🍓 V_003 (1)	\Home\Bld_01\Lab_01 \Weighing Room	1 dram vial	7.368 mg	0 mM	1.1891 m
	🗏 🗌 🍈 <u>V 003</u>	\Home\Bld_01\Lab_01 \Weighing Room	1 dram vial	7.368 mg	0 mM	1.1891 m

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

Stream # 1 - Dispense a	nd Solubilise into Tubes for Delivery
Parent:	0 🗸
Recipient:	Ash, Alice (Administrator)
Destination Location:	\Home\Despatched V
Despatch CC:	cro@corpmail.com
Amount:	Min: 400 Target: 500 Max: 600 µL 💙
Concentration:	10 mM 🗸
Solvent:	100 % DMSO 🗸
Bottle Type:	2D Mini Tube (1.4 mL) 🗸
Containing Labware:	(None) V
Apply Changes	

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	<u>19</u>
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.







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

Orders						
	Barcodes					
View Order Orders Create Order	Generate 5 Barcodes	Barcode(s) from Rang	Mosaic Barco	des (B000000000 - B9999	99999)	-C
Inventory	- O ta Mile					(0 items entered)
View Labware Item View Substance	Details			Contents	_	
Import / Update Create Substance	Labware Type:	* 2 dram vial	~	Substance Type:	Small Molecule	
Create Rack/Box Generate Barcodes Print Labels Sets	Expiry Date:	(Select one) 1 dram vial 2 dram vial 2D Mini Tube (0.5 mL)	12	Substance:	CompoundBab D ID	ch d10c1 -
Lists	Thaw Count:	* 2D Mini Tube (1.4 mL)			Name	1
Stores Automated Stores Locations	Comment:	2mL CryoVial Delivery Vial (10 mL) HR Tube (2.5 mL) Storage Tube (15 mL)	$\hat{}$	Total Thaw Count:	• 0 • nL	▼ Measured ▼
My Pick List My Place List		Storage Tube (50 mL)		Concentration:		

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

i Mosaid	Inventory Se	earch	
Orders	🚱 Open Saved Search ∓	Save Search Ŧ	View recent searches
View Order Orders Create Order	Search: Tubes - Find Ven		۲
Inventory	- 🍦 Add Parameter:	×	
View Labware Item View Substance Import / Update Create Substance Create Rack/Box Generate Barcodes Print Labels Sets Lists	Amount Vendor Labware Type Location Search	> 5 mg * Contains MerAT * * = HR Tube (2.5 mL) * * = Home\Vial Store * *	· · ·
Stores Automated Stores Locations My Pick List My Place List Search/Report Inventory Search			

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.



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

Date	Event	Item	Order	Run	Operator	Machine	Workstation	Operation	Description	Reason For Change
From										
o Tilter	[All]	[AII]	[All] 💌	[IIA]	[A]] 💌	[All]	[All]	[All]		
						Manual			B00000001 created with the following properties:	
(2/29/2016 4:12:02 PM	Created	B000000001	20	100006	DEMOMOSAICS	Weighing		Dry Dispense	 labware type set to '2D Mini Tube (1.4 mL)' thaw count set to 0 	<u>.</u>
2/29/2016 4:12:02 PM	Requires Secure Storage Set	B000000001	20	100006	DEMOMOSAICS	Manual Weighing	2	Dry Dispense	B000000001 does not require secure storage	2
2/29/2016 4:12:02 PM	Added	B000000001/A01	20	100006	DEMOMOSAICS	Manual Weighing	<u>.</u>	Dry Dispense	0.784 mg (M) of substance transferred from <u>d13t3/A01</u> to <u>B000000001/A01</u>	a)
2/29/2016 4:12:03 PM	Moved	B000000001	±1	100006	DEMOMOSALCS	Manual Weighing	*	-	B000000001 was moved from '\Home' to '\Home\Bld_01\Lab_01\Weighing Room'	\$3
2/29/2016 4:13:25 PM	Diluted	B00000001/A01	20	100007	DEMOMOSAICS	Liquid Handler 1	÷	Solubilise	249.857 µL of "DMSO" at 100% added to B000000001/A01	₹.
2/29/2016 4:13:25 PM	Moved	B000000001	2	100007	DEMOMOSALCS	Liquid Handler 1	-	2	B000000001 was moved from '\Home\Bld_01\Lab_01 \Weighing Room' to '\Home\Bld_01\Lab_01\Liquid Handling Room'	2
2/29/2016 4:13:43 PM	Despatched	B00000001	20	\$.	DEMOMOSAICS		169.254.249.1	Despatch	B00000001 despatched	¥.
2/29/2016 4:13:43 PM	Moved	B000000001	20	<i>t</i> :	DEMOMOSAICS	-	169.254.249.1	-	B000000001 was moved from '\Home\Bld_01\Lab_01 \Liquid Handling Room' to '\Home\Despatched'	5
									Clear Filters Save Column Settin	gs Restore Default Column Setting

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

Login Name 👉	<u>First</u> <u>Name</u>	<u>Last</u> <u>Name</u>	Description	Email Address	Show Inactive
Administrator	Alice	Ash	Administrator	alice.ash@titian.co.uk	Active
olivia.owen	Olivia	Owen	Operator	olivia.owen@titian.co.uk	Active
raymond.roberts	Ray	Roberts	Recipient	raymond.roberts@titian.co.uk	Active
roger.ruskin	Roger	Ruskin	Requestor	roger.ruskin@titian.co.uk	Active

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

Figure 12: Selection of role permissions

Details			
Role Name Administrator			
Status: • Active	~		
Save GUndo			
Users with Role	Permissions for Role		
Administrator (Ash, Alice)	Can approve any restriction Can be an order output recipient Can create and edit Substances Can create manual stores Can create order templates Can create orders of any type Can create persistent orders Can create restrictions	^	
	Can create sets Can create stream templates	~	
🖗 Add 🛛 🎉 Remove	Add 😹 Remove	Add KRemove	
	(Select One) Can create folders	OK	
	Can manage shared orders Can unlock any list		



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

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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



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