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Storage Buffer Compositi Tag Location Test Property

#### ABSTRACT

Small molecule (MW<1200) compound management teams typically have the responsibility of managing inventory of a large number of molecules that have been provided by the medicinal chemist. The compound management group, depending on the infrastructure, distributes these small molecules as powders or solutions and may even create the assay-ready plates necessary for biological testing. The Inventory Management group within a biologically oriented company such as AssayQuant has a different set of challenges compared to the traditional small molecule Compound Management lab. As an assay service provider, AssayQuant relies not only on robust inventory tracking of its small molecule customer compounds, but also on various components of the assay including the *PhosphoSens®* substrates, enzymes, and reagents necessary for a multitude of different workflows and users, while ensuring sufficient inventory to meet all needs. AssayQuant has developed and implemented an inventory management system that supports the inventory necessary for maintaining biological assay testing and satisfying the requirement of the finance team to track cost of goods. The inventory management system, developed in collaboration with Scigilian, relies on four distinct inventories: PhosphoSens® substrates, enzymes, customer compounds, and reagents. A registration system was developed that allows the scientist to properly register the individual entities with the annotations required for the downstream data analysis. Included within the registration system is the capability to maintain the individual Certificate of Analysis documents that are required for each of the *PhosphoSens*<sup>®</sup> substrates. Although each inventory is tracked and maintained uniquely, the entire inventory management system is encapsulated into one overarching software platform that enables registration, storage, ordering, retrieval and reconciliation of the inventory required for testing, followed by a seamless transition of information into the data analysis portion of the software to provide documentation support and traceability for the final data set.



Peptide sequences are synthesized using solid-phase methods with the Sox fluorophore coupled through the sulfhydryl group of a cysteine residue proximal to a protein kinase phosphorylation site, such as a tyrosine, serine or threonine. Upon addition of a kinase, the peptide is phosphorylated. In the presence of magnesium ion, a chelation complex is formed with the phosphate group, resulting in fluorescence enhancement of the Sox fluorophore that can be monitored continuously as fluorescence intensity (A). Kinase inhibitors prevent phosphorylation and thus fluorescence. At any point, Europium ion can be added, to displace the magnesium ion, resulting in a long wavelength, time-resolved fluorescence (TRF) endpoint/Red format (B) that is useful for high-throughput or structure activity relationship (SAR) applications.

#### **INVENTORY FOR ASSAYQUANT'S SERVICES**



• The Inventory Management group also needs to track all compounds submitted by client. • The accountants need to understand the cost of all the inventory.

# AssayQuant<sup>®</sup> Multiplexing Inventory Management: Satisfying the Enzymologist, the **Customer and the Executive Leadership Team**

- software to allow for consistent experimentation Earl May, Ph.D Sr Director of Discovery **Fechnologies** Store

Scigilian Re	EQUEST Invento	ory Assays - Req	uests - Dispatches	Reports - Resources -			Find requ	iest by key	
	es 					Create Assay R	lequest Cr	reate Compound Re	ques
Row Search Term	Search Option	Parent	Compound	Batch/Plate Set	Store Item	Cmpd, Wt. (o/mol)	Salt Name	Total Amt. Solid	N
1 S-000003001	COMPOUND	S-000003001 @	S-00003001-000 @	S-00003001-0000001 ĝ	-	200.00			
					T000037053	200.00			
					T000062210	200.00			
				S-000003001-000X002 🔒	+	200.00			
		_	S-000003001-001	S-000003001-001X001	+	200.00			
2 S-00000002	COMPOUND	S-00000002	S-0000002-000	S-0000002-000001	+	200.00		5,000.00 mg	5,
3 S-00000103	COMPOUND	S-00000103	S-00000103-000	S-00000103-0000001	+	200.00		5,000.00 mg	5,
4 S-00000104	COMPOUND	S-00000104	S-00000104-000	S-00000104-0000001	+	200.00		5,000.00 mg	5,
5 \$-00000105	COMPOUND	S-00000105	S-00000105-000	S-00000105-000X001	+	200.00		5,000.00 mg	5,
6 S-00000105	COMPOUND	S-000000106	S-00000106-000	S-00000106-0000001	+	200.00		5,000.00 mg	5,
7 S-000000107	COMPOUND	S-000000107	<b>\$-000000107-000</b>	S-00000107-000X001	+	200.00		5,000.00 mg	5



Request

- All inventory is tracked with the Scigilian platform
- Unique customization of the data analysis algorithm was developed simultaneously.
- See poster (1027-D) Automated Linear Range Determination and Applications to Enzymatic Progress Curves

			SA	TISFY	ING THE LEA	DERSHI	P				
							Erik Sc Co-founder, P	chaefer, Ph.D. Gerry I President, CEO, CSO Chief Finan	abonte Michelle Lyles, Ph.D. cial Officer VP, Commercial Operations	Director of Operations	Earl M Sr Dir Disc Techr
<ul> <li>Additional fields within Scigilian Store were developed to track the cost of the materials</li> </ul>				t	Enzymes	Sens Pepti	sor des	Compounds	Reagents (i.e ATP, DTT, EGTA)	Labware	
<ul> <li>Material Costs are trackable down to the container level.</li> </ul>					Source Vial Cost	Synthesi	s Cost	Reagent costs	Chemical Costs	Plate Costs	
<ul> <li>Cost of Goods reports are exportable for the accountants to analyze</li> </ul>					Custom Testing Labor	Fmoc Cy Cos	ys Sox st	Labor Cost	Labor Cost	Vials/tubes	
		Cost Report			Profiling Labor Costs	Labor (	Costs			Cost	
Upload Maps		Inventories Search By Peptide Inventory   Barcode	Search Value Search Advanced Search Clear		Labware costs	Labwar	e Cost	Labware costs	Labware costs	Pipette tip cos	st
Column Order	Hidden Fields	Barcode ↑	Batch Id	Cost (\$)	Labware costs	Labward	CUSI				
Move Optional Fields Drag to rearrange and/or hide fields.	Comments	TST000001	AQT0101-00003-01	N/A							
Add Blank Field	Compound Molecular Weight	TST000002	AQT0101-00003-01	N/A							
1. Barcode *		TST000003	AQTST24-001-01	\$10.47			Entity: Sensor Pept	tides (Sensor Peptides)			Edit
2. Position *	Container Type Name	TST000004	AQTST24-001-01	\$10.47			Properties				+ Add Property
3 Sample Name *	Diluent	TST000005	AQTST24-001-02	\$10.47			Name	Type	true	Included in Uniqueness Check	Ň
	Freeze Thaw Count	TST000006	AQTST24-001-03	\$10.47			Class	Text	Sensor Peptide, Phosphopeptide, Peptide true	false	1
4. Amount *	Heated	TST000007	AQTST24-001-04	\$10.47			HPlus	Text	true	false	1
5. Concentration *		TST000008	AQTST24-001-05	\$10.47	_		Mol Wt	Number	Molecular Weight true	false	<i>`</i>
6. Cost Per Mol				\$10.47			Rs Volume	Number	L to solubilize 1mg to 1mM true	false	i
	Inventory Set Name	TST000010	AQTST24-001-07	\$10.47			Sequence	Text	true	false	i
	Location			Items	per p	_					

## **INVENTORY MANAGEMENT**



Example

#### • The registration of kinases must be segmented to encompass the variety of kinases that are available from

	encompass the variety of kinases that are available from	Sensor Peptides	[AQT][Base]-[Lot]-[Source]	Batch ID: AQT0101-55555-01
	the different kinase suppliers		AQT1234-12345-12	Substance ID: AQT0101
	the unreferre kindse suppliers.	Customer compounds	[CPD][Base]-[Salt]-[Batch]	Batch ID: CPD000001-00-0001
			CPD123456-12-1234	Substance ID: CPD000001
•	Additional kinase variations need to be assessable in the	Enzymes	[ENZ][Base]-[Mutant]-[Tag]-[Vendor]-[Lot]	Batch ID: ENZ0001-001-01-
	software to allow for consistent experimentation		ENZ1234-123-12-123-1234	001-0001
	soltware to anow for consistent experimentation.			Substance ID: ENZ0001-001-01
		Reagents	[RGT][Base]-[Salt]-[Lot]	Batch ID: RGT00001-01-000001
			RGT12345-12-123456	Substance ID: RGT00001-01

# • AssayQuant's sensor peptides require sequence

- synthesized peptide.
- within the inventory.

### SATISFYING THE ENZYMOLOGIST & THE CUSTOMER

SCIGILIAN							
			Raw Assay Data	Ar			
Approve     Dany       autification     Invertory       orgat     Please       logat     Please       logat     Please       o     o       logat     Please       logat     Please       o     o       logat     Please	drequet by key       ▲ The Biologist          ☆       ▲         ☆       ▲         Hatstanding Issues          •       Provider Assignment 1 for Sciglian Assay         •       Scheman 1 for Sciglian Assay         •       Scheman 1 for Sciglian Assay         •       Devider Assignment 1 for Sciglian Assay	Matrix Socialica Data: Conver [304]49.455223	a       y       a       a       in       in<	Cortige Control     Contro     Control     Control     Control     Contro			
Sample Log         Al           0         0         0         0           0         0         0         0         0           15         216         740         0         0           0         0         0         0         0         0           0         0         0         0         0         0         0           0         0         0         0         0         0         0         0           101         103         2         53         0         0         0         0         0         0           0         0         0         0         0         0         0         0         0	ssay Order Item Queues Say Order Item Queues Provider A Date Order Provider A Date Order Sogliten Assay 1955 40			Ubtom 1 =           Connet         Source 1 as           sipa         -0.07			

• Singular software platform allows for seamless transition from container inventory (Store) to physical assay to data analysis (Analyze, Visualize).

### **SUMMARY**

• Inventory Management group at AssayQuant developed, in collaboration with Scigilian, a software platform that manages all of AssayQuant's inventory. • Unique inventories were developed to encapsulate the multiple inventory types the inventory management group is required to maintain (kinases, peptides, small molecules). • Unique registration segments were developed to better categorize the kinases and AssayQuant's sensor peptides.

• Cost of Goods tracking at the container level was also developed as mandated by the leadership team so that metrics surrounding profit margins could be generated



Description	Required
	true
Sensor Peptide, Phosphopeptide, Peptide	true
	true
Molecular Weight	true
Solvent for solubilization	true
uL to solubilize 1mg to 1mM	true
	true

# annotation instead of a chemical structure. Sensor peptide supplier (source) code is necessary for a Client compounds need to traceable and segregated



