

Multiplexing Inventory Management: Satisfying the Enzymologist, the Customer and the Executive Leadership Team

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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*[®] 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.

INVENTORY MANAGEMENT

Enzymes	Sensor Peptides	Compounds	Reagents
MW: >20,000 M _r	MW: 1000 to 3500 M _r	MW: <1500 M _r	MW: <1500 M _r
Liquid	Solid or Liquid	Solid or liquid	Solid or liquid
Conc: µg/mL	Conc: mM	Conc: mM	Mixtures or individual solutions
AQT or Customer owned	AQT owned	Customer owned	AQT created or purchased
-80 °C storage	-20 °C storage	-20 °C storage	Room temp or -20 °C storage

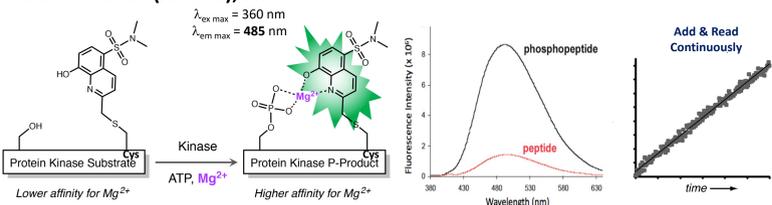
- The registration of kinases must be segmented to encompass the variety of kinases that are available from the different kinase suppliers.
- Additional kinase variations need to be assessable in the software to allow for consistent experimentation.

Entity	Format	Example
Sensor Peptides	[AQT][Batch] [L][S] [Source]	Batch ID: AQT0101-5555-01 Substance ID: AQT0101
Customer compounds	[CPD][Batch] [S][W] [Batch]	Batch ID: CPO000001-00-0001 Substance ID: CPO000001
Enzymes	[ENZ][Batch] [Mutant] [Tag] [Vendor] [L][S]	Batch ID: ENZ0001-001-01-001-0001 Substance ID: ENZ0001-001-01
Reagents	[RGT][Batch] [S][W] [L][S]	Batch ID: RGT00001-01-000001 Substance ID: RGT00001-01

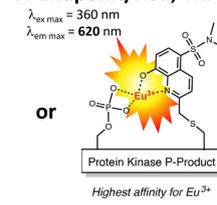
- AssayQuant's sensor peptides require sequence annotation instead of a chemical structure.
- Sensor peptide supplier (source) code is necessary for a synthesized peptide.
- Client compounds need to be traceable and segregated within the inventory.

THE PHOSPHOSENS[®] ASSAY – CONTINUOUS & ENDPOINT/RED FORMATS

A. Continuous (Kinetic), FI

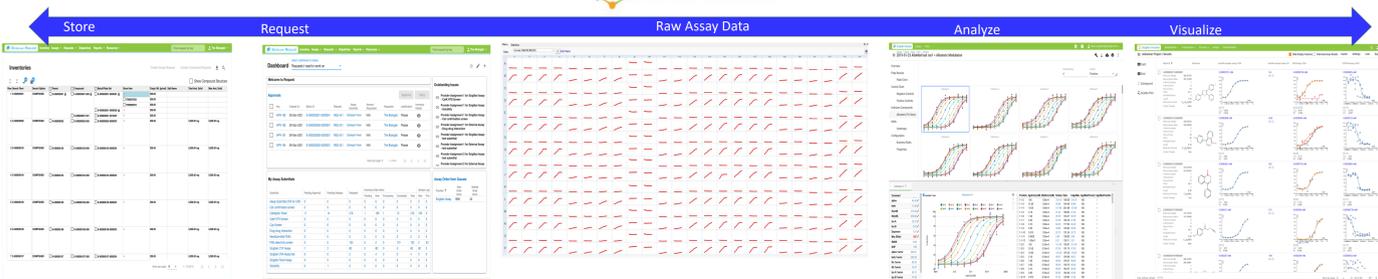


B. Endpoint/Red, TRF



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.

SATISFYING THE ENZYMOLOGIST & THE CUSTOMER

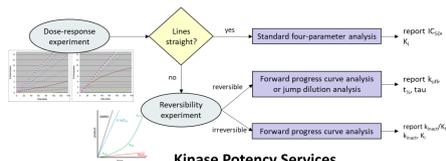
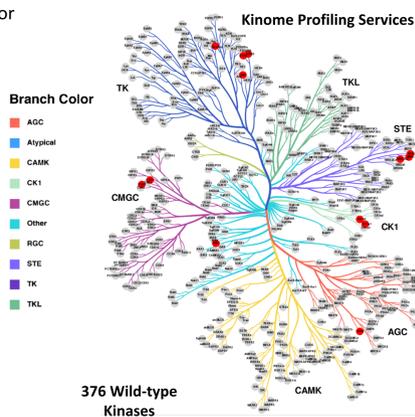


- All inventory is tracked with the Scigilian platform
- Singular software platform allows for seamless transition from container inventory (Store) to physical assay to data analysis (Analyze, Visualize).
- Unique customization of the data analysis algorithm was developed simultaneously.
 - See poster (1027-D) *Automated Linear Range Determination and Applications to Enzymatic Progress Curves*

INVENTORY FOR ASSAYQUANT'S SERVICES



- Sensor Peptide Inventory needed for
 - Catalog Sales
 - Kinome Profiling Services
 - Kinase Potency Services
 - Custom Assay Development
- Enzyme Inventory needed for
 - Catalog Sales
 - Kinome Profiling Services
 - Kinase Potency Services
 - Custom Assay Development



AQT PhosphoSens Platform

Sensors & Sensor Peptides

Enzymes (Targets)

Compounds

Reagents KRB, EDB, ATP, DTT

Labware

Data

- The Inventory Management group needs to maintain all the components that are required for the *PhosphoSens*[®] platform to function.
- The Inventory Management group also needs to track all compounds submitted by client.
- The accountants need to understand the cost of all the inventory.

SATISFYING THE LEADERSHIP



- Additional fields within Scigilian Store were developed to track the cost of the materials
- Material Costs are trackable down to the container level.
- Cost of Goods reports are exportable for the accountants to analyze

Enzymes	Sensor Peptides	Compounds	Reagents (i.e. ATP, DTT, EGTA)	Labware
Source Vial Cost	Synthesis Cost	Reagent costs	Chemical Costs	Plate Costs
Custom Testing Labor	Fmoc Cys Sox Cost	Labor Cost	Labor Cost	Vials/tubes Cost
Profiling Labor Costs	Labor Costs	Labware costs	Labware costs	Pipette tip cost
Labware costs	Labware Cost	Labware costs	Labware costs	

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.

