Developing and Embedding In-House Compound Management within Artios





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Introduction

Design, Make, Test and Analyse (DMTA) screening requires the generation of compound assay ready plates (ARP) a process that can be slow, costly and resource intensive.

Negative impact on project cycle times/resource burden.

Using dedicated software and automation, we have developed in-house compound management (CM) for DMTA processing and plate generation:

Audited and trackable process – increased

Artios In-House Compound Management Workflow

Compounds prepared as DMSO solutions and imported into Mosaic Sample Bank system/compound collection.

Mosaic Sample Bank System

Full sample data and storage information / compound ordering and assay plate generation / tracking of compound usage and assay plate maps for analysis

Sample information

"Sample Processing" Re-format / Dispense / Serial dilution and Replication into final assay plate(s)

Analysis, posting

- sample/data integrity.
- Fully automated workflow for biochemical & cellular assays.
- Reduced cycle times/cost.
- Faster data reporting to drive decision making/more effective use of resources.

Benefits of In-house CM Plate Supply

External Plate Supply/Logistics

Legacy Sample Registration to Test date (Typically Assay Ready Plates from CRO)





CM Plate Generation Quality

Biochemical/cellular assays demonstrated comparable compound activity/assay quality.







800nL dispensed in each well (1% DMSO)

Project B Typically >3 weeks (Up to 50 days)



Cost of Assay Ready Plates

anacy external and internal cost for plate generation

DMTA Cycle Times

Up to 40 % reduction in median cycle time (registration to data posting).

In-House CM Workflow Details (*)

Registration to Shipping at CRO - typically 1 day Shipping from CRO to Artios - typically 7-10 days Assay Ready Plate generation to Data posting - typically 1-2 days

Compound registration to Data Posting

Legacy assay ready plates supply process (Days)*	21
In-House CM assay ready plate supply process (Days)*	13

TR-FRET Probe Displacement Assay



TR-FRET Assay



* Based upon typical Biochemical assay

CRO (External)	Artios Legacy (Tecan D300e)	In-House CM
£600	£300	£35(*)

(Based upon 30 compounds per 384 well assay plate) *(following repaying of initial costs)

- Reduction in cycle times and cost due to direct supply to Artios.
- Increased sample control and tracking due to sample management system.
- Generation of assay plates for DMTA, Kinetic & Mechanistic formats.
- Automated workflows and analysis integration reduces human intervention.

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Summary and Future Applications

Developed and embedded end-to-end workflow for sample storage/tracking, requesting, processing, plate generation and sample maps for analysis.

- Manage sample requesting and fulfilment of orders from our centralised on-site stores, with full inventory tracking and workflow management.
- Sample pick and generate assay ready plates for both 96 and 384 well assay formats, including DMTA, Kinetic and Mechanistic formats.

Results in faster plate generation and screening, quicker data reporting to drive decision making and effective use of resources (both financial and FTE)).

- "The compound management system has definitely" been a big positive and aligns us with industry standard"
- "The CMG has definitely had a positive impact.....We are now receiving compounds from the CRO and typically getting results from the FRET assay by the end of the following day (sometimes same day!)"

Additional use for Mosaic / automation e.g. CMC sample tracking / high throughput reagent generation / protein crystallography