

## Assay Requesting at Roche

Titian Mosaic software user, Roche, has further enhanced the efficiency of its preclinical drug development process with the new Assay Requesting module.



As a multinational healthcare company, Roche commands the skills of thousands of scientists around the globe, each determined to advance the understanding and treatment of diseases through the development of innovative new compounds.

Coordinating the work of such a broad range of scientists and managing large and ever-expanding compound libraries (approximately 1 million dry powder and more than two million solubilised compounds, a typical inventory for a pharma company of Roche's size), does not come without its challenges. Novel compounds are created and transferred between departments to test different properties. This complex network demands precise coordination, and efficiency becomes the number one priority to keep the process running smoothly. By installing Titian's Mosaic sample management software with the Assay Requesting module in 2013, Roche has further streamlined how its multi-disciplinary team requests a large variety of compound assays, translating to significant improvements in terms of ease-of-use, reagent savings and most importantly – efficiency.

The system deployed currently supports all preclinical small molecule research projects involving approximately 500 scientists and technicians across Roche pRED's (Pharma Research and Early Development) chemistry, biology and pharmacology teams in Basel, Switzerland. On an average working day, this means dozens of newly synthesised compounds are entered into the system, hundreds of compound orders are processed and thousands of microtiter plate wells are filled.

### Easy integration

While the initial high-throughput drug discovery phase typically involves a uniform assay specification, automated to screen hundreds of thousands of compounds to create a hit list, the secondary screening stage focuses investigations on this smaller but targeted hit list. These promising compounds are taken through in-depth, high-value investigations for detailed characterisation of their chemical, biological and toxicological properties. This secondary screening stage is highly complex, involving many different assays on the same compound and the same assay on many different compounds.

As Dr Achim Grenz, Compound Library Manager, Small Molecule Research at Roche pRED, says: "Multiple chemists may synthesize novel compound analogues and pass these through to biologists and pharmacologists for profiling every day. The biologist might receive these submissions on different days and will have to reformat the different submissions for a single assay, resulting in duplication of effort and inefficiency. In 2008, Roche pRED introduced a central service function to support scientists in re-formatting their sample submissions. Implementing Titian's Mosaic software with the Assay Requesting module in 2013 allowed us to further improve the process and efficiency in this phase of drug discovery."

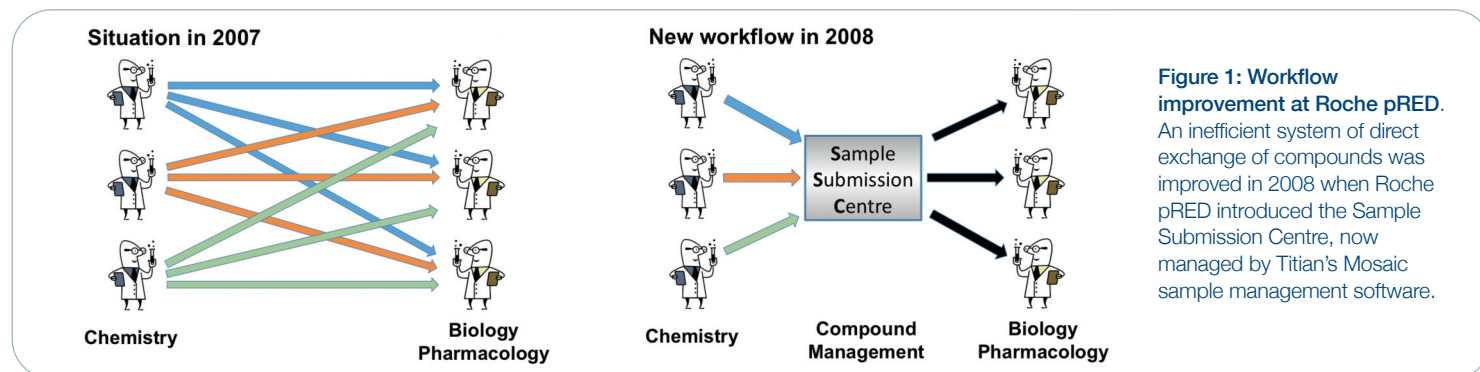
### Working together at Roche pRED

- **Chemists** generate multiple analogues of compounds from the hit list for testing.
- **Biologists** assay the new analogues for binding affinity, solubility etc.
- **Pharmacologists** further test promising compounds for biologically relevant properties, for example toxicological effects.

Compounds passing these tests have the potential to enter *in vivo* testing.

### Efficiency gains in drug discovery at Roche pRED

The complex process of drug discovery has been streamlined at Roche pRED over a number of years. In 2008 there was a complete restructuring of the process of secondary screening from a direct exchange of compounds between multiple chemists and biologists to a new centralised workflow (Figure 1). With initial roll-out of this workflow at its Basel site, all compounds developed by Roche pRED's medicinal chemists were entered into a "Sample Submission Centre" (SSC). Use of the SSC enabled chemists to enter and log novel compounds into a centralised system using custom software. These compounds could then be accessed by biologists, allowing them to set up assays more efficiently.



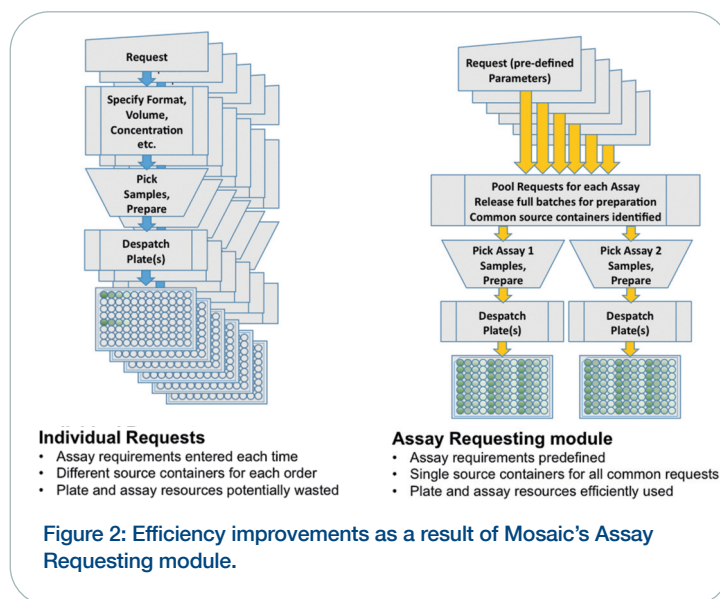
**Figure 1: Workflow improvement at Roche pRED.** An inefficient system of direct exchange of compounds was improved in 2008 when Roche pRED introduced the Sample Submission Centre, now managed by Titian's Mosaic sample management software.



In 2013, the Roche pRED team brought in Titian's Mosaic sample management software, with the Assay Requesting module, to further improve efficiencies, particularly by tackling the assay requesting aspect. This allowed all aspects of sample management to be tracked and managed within the established and reliable software solution, integrating with automated systems, where required. Mosaic has enabled Roche pRED to track the entry of compounds from all chemists into the inventory, manage requests for a variety of profiling assays and ensure compounds are correctly formatted for delivery for assay.

## Assay Requesting at Roche pRED

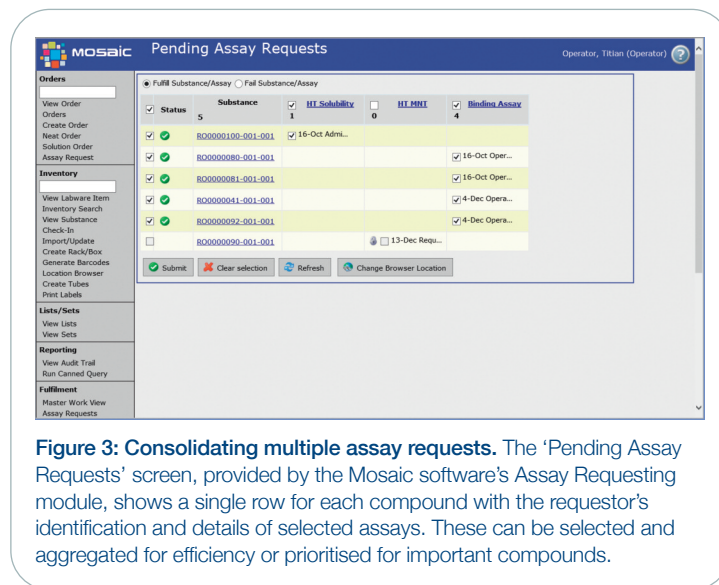
The implementation of Mosaic has improved the efficiency of compound tracking and management. The addition of the Assay Requesting module has provided a simplified and streamlined workflow for assay requests, making the most effective use of a requestor's time. For Roche pRED, the software was set up with around 100 frequently used assay types pre-defined with delivery format, volumes and plate layout, including serial dilution plates.



Requestors are able to select specific assays quickly and efficiently using the easy-to-use interface without needing to have specialist knowledge of all assay parameters. The Assay Requesting module also delivers live feedback on selected assays, providing alerts on potential duplications, checking compound availability and any provisioning requirements on the requestor's screen. The intuitiveness and ease-of-use is evidenced by the fact that, following an initial series of training sessions, existing Mosaic users have been able to train new users themselves.

At Roche pRED, the Assay Requesting module also allows a Mosaic operator to prioritise and aggregate all assay requests. Alternatively, at other companies, it is possible for individual assay owners to use the

Assay Requesting module to manage relevant requests at their respective locations. By moving away from an 'as-required' approach, fewer individual assay runs are required and more complete assay plates are processed for a given batch of requests. This reduces reagent and consumable waste and leads to efficiency gains for the biologists in the laboratory.



**Figure 3: Consolidating multiple assay requests.** The 'Pending Assay Requests' screen, provided by the Mosaic software's Assay Requesting module, shows a single row for each compound with the requestor's identification and details of selected assays. These can be selected and aggregated for efficiency or prioritised for important compounds.

It is regularly the case that two or more chemists submit compounds for the same assay at different times. With Assay Requesting, multiple requests from different chemists can be aggregated, resulting in more efficient use of time, consumables and equipment in the compound management facility. The Assay Requesting module allows this to be achieved by providing a summary view of all assay requests (Figure 3), permitting the Mosaic operator to select and process or defer until more requests are received. At Roche pRED, this system allows a guaranteed maximum turnaround time of 36 hours for any given request no matter what delivery format is required, with the option to prioritise specific requests, as needed.

## Conclusion

Between 2008 and 2014, the drug discovery process at Roche pRED underwent a progressive evolution to enhance efficiency. The latest improvement has been the implementation of Titian's Mosaic software with the Assay Requesting module, and this has provided significant efficiency gains throughout the secondary screening stage through simple selection and aggregation.

Supporting around 500 users and more than 5000 assay requests per month, the compound processing rates achieved by the company are accomplished with approximately 3 FTE laboratory personnel. With the demonstrable success of Mosaic Assay Requesting at its Basel site, Roche is preparing to implement Mosaic at its Shanghai site later in 2014.



**Titian's Mosaic sample management software with Assay Requesting:**

- Intuitive and easy to use
- Saves time
- Minimises reagent use and waste

As the team at Roche say:  
'One Assay, One Compound, One Click'.