C+S M13 | Compound & Sample Management Summit

4 valuable ways technology in your compound management workflow will benefit you

Developing new drugs comes with the need to test compounds, often in the millions in the case of larger pharmaceutical drug discovery set-ups. Starting with screening, onto lead development, automated compound management has been on an evolutionary path. Knowing the importance of a good compound management practice to support the research and development phase of drug discovery is non-negotiable to success. But how have things changed in 2017, with technologies taking us to anywhere we want to go on the automation-to-artificial-intelligence spectrum? What are the secrets to incorporating technology in compound management workflow in a way that makes sense? And perhaps more importantly, what are the benefits we, as an industry, can expect to see?

> **The biggest differentiator between pharmas is the equipment used and IT resources, but this is a small world, and we are using similar processes and workflows — Astrazeneca**

INNOVATION

The industrial revolution we are in the midst of, which brings information technology and robotics into the laboratory, has taken innovation in drug discovery to a whole new level. In today's world, where we've moved seamlessly from processing thousands of compounds to **processing millions,** we've got all new deliverables that require us to bring flexibility. And we've risen to the challenge as an industry!

Today we can 'mix-and-match' compounds, like open-ended children's toys, into an almost infinite number of permutations and combinations. This is how we hope to find the next **'wonder drug'** - the cure to cancer; definitive relief from the common cold! That is the innovator's dream, and technology has moved us steadily forward to a place where these things are possible in shorter time frames than they ever were before. With informatics, huge sets of data are collected and, robotics can run tests on thousands of compounds, sometimes all at the same time, with **manufacturing-like precision** and **efficiency.** Artificial intelligence can take analytics to a whole new level, offering insights that fuel innovation.

Even issues of smaller sets of valid data are being addressed by scientists like this Stanford chemistry professor, who believes that ‘a relatively new type of deep learning might be the answer to AI’s low-data problem.’ This kind of machine learning is called ‘one shot learning’.

‘One-shot learning has been used successfully for image recognition and genomics, but applying it to problems relevant to drug development is a bit different. Whereas pixels and bases are fairly natural types of data to feed into an algorithm, properties of small molecules aren’t. To make molecular information more digestible, the researchers first represented each molecule in terms of the connections between atoms. This step highlighted intrinsic properties of the chemical in a form that an algorithm could process.’ When tested on different datasets, they found that they were able to make viability predictions that were more accurate.

COST SAVINGS

Managing compounds using a technology brings with it several costs - **equipment, space, people** and the costs of **keeping your sample banks running,** like ongoing maintenance and consumables. While that seems like a lot at first glance, the best way to make sure your investment is bringing you the desired returns is to think about those costs in terms of the greater efficiency it brings you. Compound management technology spells speed, which **mitigates delays** and offers **opportunity gains in bringing innovative, and much needed, drugs to market.** That is the business case for technology in compound management in itself! Add to that the fact that drug discovery technology the world over is forecast to grow considerably over the next 5 years. New platforms and exciting new possibilities for data analysis bring fresh opportunity for lead identification. This comes with the promise of storing and analyzing vast data sets at much lower costs. How? Well, economies of scale, for one. The wider adoption will drive down the cost per 'adopter', already making entry an option for more than just the very top tier. And the introduction of new players will bring competition into the market, further bringing value to the end customer.

MODEM OPERATING MODELS

Much is changing in the way compound banks are managed today. Pharma has long outsourced key parts of its supply chain for efficiency, and that thinking is makings its way over to the management of compounds as well. As far as 6 years back, Bernard Munos made waves when he suggested that Big Pharma should cut R&D to make its operations leaner. *"Several pharmaceutical companies (including some of the very largest) are already experimenting with an increasingly outsourced research model, creating their own virtual drug discovery groups with a lean internal staff, and relying on external service providers to do the bulk of the heavy lifting."*

Outsourcing in compound management can be an efficient operating model from a resource and effort perspective. While Pharma is no stranger to this even within compound management, in the past, the model has been used primarily to bring in short term capacity. The model, however, is a good one. First, because people who already have the technology will charge you as part of your operating expenses rather than as capital expenditure. With outsourcing you are will also likely benefit from more updated technology because the operators of the labs will be more current, in hardware and software, than individual organizations can hope to be.

This, combined with the implications of lower technology costs overall, firmly tilts the pitch into one that is much more easily accessible.

QUALITY & FLEXIBILITY

The process of compound management has a viable shortlist at its core. Millions of compounds are tested and narrowed down to a smaller set for optimization. A key focus for drug discovery in recent years has consistently **better quality** (in the target and screening of compounds) and **greater flexibility**. The first is brought by the use of different screening approaches and the **stability** and **speed** that can come from using technology. And the second has seen many new models in recent years. One example of an idea that is **bringing greater flexibility and efficiencies is the use of modularity in storage and transportation**. Samples are stored in automated shelving that can be moved/increased/decreased to suit changing needs. Retrieval from these shelves can either be manual or fully automatic. Another is innovative packing methods – several options including the use of compression, air, and virtual reality now exist. And from a workflow perspective,

an example of the kind of flexibility and precision that exists can be seen in the way in which compounds are ordered today. Many sample management service providers offer software that allows customers to check the availability of compounds, choose the types of containers needed for delivery and storage, and customize protocols for regulatory needs.

The high-throughput environment of compound management is integral to the drug discovery world. Quick, and accurate, processing is the goal, and in recent years, nothing has delivered those values like technology has.

For more information on what technology, in any operating model, can do for your compound management facilities, please take a look at the **13th Compound and Sample Management Summit in Philadelphia** from **August 28-30, 2017.**

The following sessions will bring value to those considering implementing, or upgrading to, new technology for greater efficiency:

IMPLEMENTING NEW TECHNOLOGY TO OPTIMIZE COMPOUND FLOW FROM REQUEST TO ASSAY



- Learn the benefits and pitfalls of rolling out a new requesting application for those on the bench
- Maximize the opportunity to evaluate how much information your organization is gathering about types of requests that stakeholders are making
- Provide a backbone for research operations by aligning request processes with other groups and goals
- Assess future flexibilities such as integration with other data management systems and with CRO partners

SPEAKER: MaryBeth Burton, Director, Discovery Sample Management, Merck

INTEGRATING AUTOMATION AND A HIGH-PERFORMANCE TEAM WITHIN A COMPOUND MANAGEMENT ENVIRONMENT



- Discuss process improvement as a balance of both automation and lab skills
- Promote staff engagement during transitions to automated operations
- Integrate CM activities with the rest of your internal departments

SPEAKER: Jefferson Chin, Senior Research Scientist, Bristol-Myers Squibb

AGENDA **PURCHASE PASS**

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(1) http://www.roboticstrends.com/article/how_deep_learning_could_help_drug_discovery/Artificial_Intelligence
(2) https://cs.stanford.edu/~woodward/papers/active_one_shot_learning_2016.pdf
(3) http://www.roboticstrends.com/article/how_deep_learning_could_help_drug_discovery/Artificial_Intelligence
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