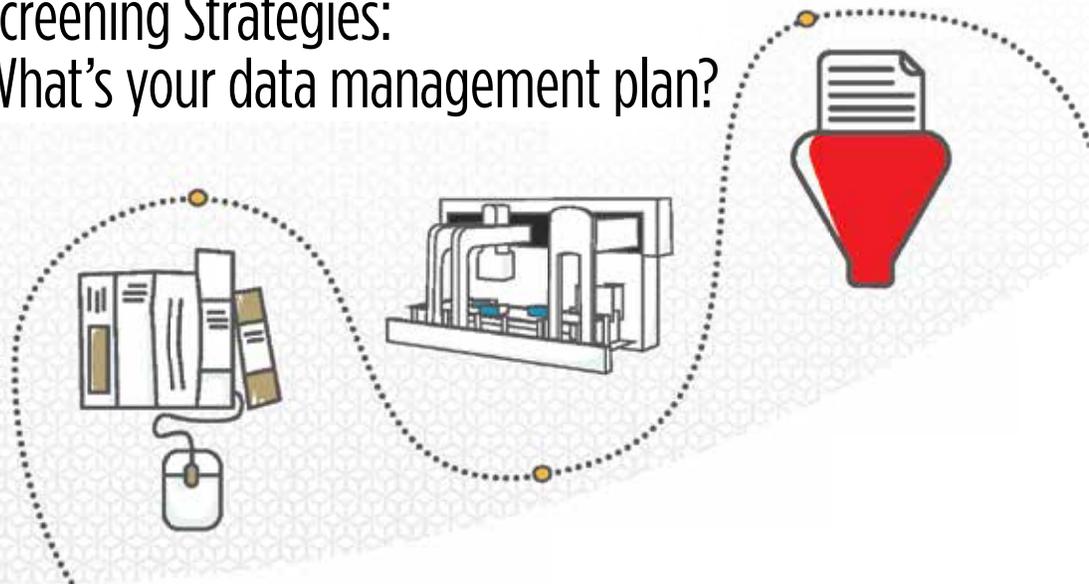




Screening Strategies: What's your data management plan?



For most scientists, secondary screening is a complicated, time-intensive, and error-prone task. That's because screening yields piles of data, and that data can be bulky and hard to migrate between platforms. Different file formats, different interfaces, different assay modalities, and different endpoints all stand between you and your data. Since most scientists screen multiple parameters sequentially or at the same time, those piles of data can go from manageable to wildly out of control in short order.

Having a plan for your data management is always a good idea, but many scientists don't appreciate the flood of data until they're struggling to keep their heads above the surface. Don't drown in your own data! Make a plan for managing and migrating your data in a proactive way. Spending a little time developing and executing a plan can result in a significant savings in both time and manpower down the line, while also improving the reliability of the screen results. To get you started, here are a few tips that can help you to implement your own data management plan - hopefully, before your next screen!



Keep it together (your data, that is)

When you use multiple, disconnected platforms for your screening assays, your data has to travel from system to system - by network, thumb drive, printout, or manual entry - or be compiled elsewhere. Every time you port your data from one system to another, you risk losing or misidentifying some of that data. Even if it's just one well that gets lost in the shuffle, your statistical analyses can be seriously impacted. Your crisp and clean data, in triplicate, are now a bit skewed. It's an inherently loss-prone system!

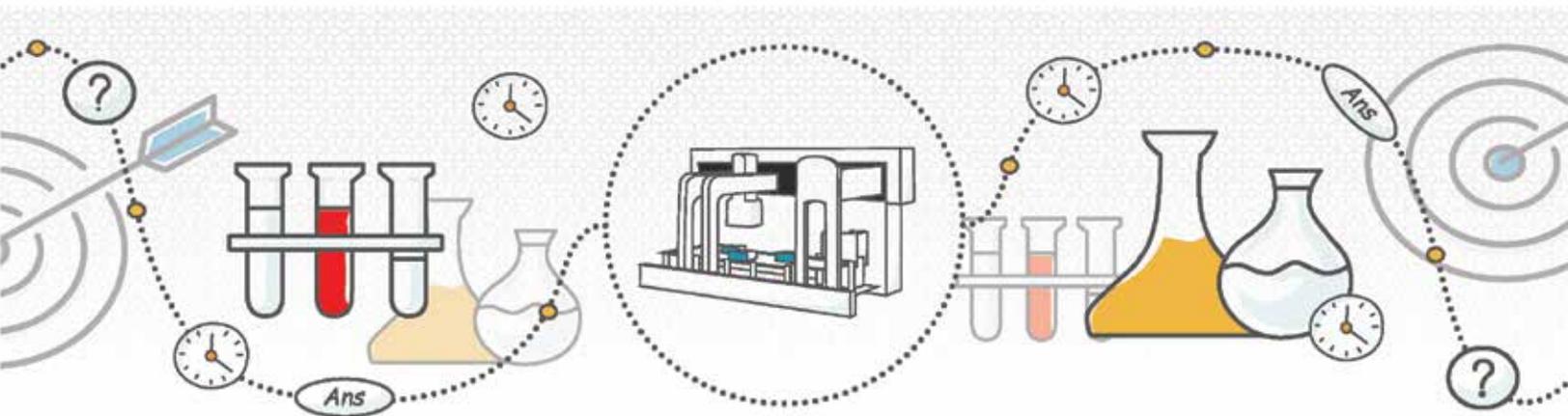
To minimize the risk of losing, misidentifying, or – worse – forgetting about your data, you'll want to have a well-defined system for how your data are handled once they're generated. Rather than dashing from machine to machine, grabbing reports (or saving files to the attached computer's desktop) before running to the next assay, you'll want to slow down a bit to make sure that your data are complete and properly cataloged before moving on to the next assay or time point. This may seem like common sense, and it is, but no one really faults someone for taking shortcuts in the middle of a 12-hour day of assays when they're getting a bit overwhelmed.

The easiest way to keep track of your data is by using integrated systems – systems that don't require manual interaction and share data between themselves. This helps in two ways – first, it cuts down on your hands-on time. Integrated systems allow you to plan ahead and program your assay flow, without needing to babysit the machines. Screen overnight, and interpret your data before lunch the next day. Second, it keeps your data together and in context. When the assay platforms share data automatically, there's no need for manual data porting, which makes it much less likely that you'll lose, misidentify, or forget about your data.

Using a scheduling and data-rich software package that can integrate your screen, whether it comprises one workstation or several, is critical for ensuring that the integrity of your data remains high. Most workstations are compatible with a few key pieces of equipment, and others can claim a bit more compatibility, but the best case scenario is to be able to automate your entire screen, from plating and growing your cells to lead optimization and beyond. If your software can't connect with all of your workstations and peripherals, you're signing up for additional hands-on work – and no one has time for that these days!

This is also a key point in the traceability of your data. When your cells travel from plate to plate, machine to machine, mistakes can be made. Optimally, you'll want to keep your cells and plates as static as possible while the assays go on around them, but when transfer is required, it's essential to have a system that automatically tracks this transfer. In this way, you can avoid mixing up or cross-plating cells.

The ultimate goal of using integrated systems for screening is to preserve the integrity of your data. As you can imagine, data that is fragmented and decontextualized can, at best, be uninterpretable and, at worst, be misleading. Don't let your hard-won data lose its value!



Choose a platform that meets your needs

Everyone agrees that automation is great, in theory, but most automation platforms are only capable of automating a fixed set of processes and procedures. What if you need to automate refrigeration, liquid handling, incubation, and luminescence detection, followed by the washing of “positive” wells so those cells could continue to the next phase of screening? Would your screening platform be agile enough to adapt to your needs? Or, what if the aims of your project change, completely altering your experimental design and endpoints? Can your platform be rapidly adjusted to avoid downtime?

Your platform should also enable you – the scientist – to access and evaluate your data without needing to call IT to write code to extricate your data from the workstation. After all, what's flexible about being on someone else's time frame? You don't want to wait for your data, and your data don't want to wait for you! Having direct access to and control over your data lets you schedule your analysis at a time that works for you, and it minimizes the chances that your files will be renamed or resorted without your first-hand knowledge. IT is always helpful, and they know their stuff, but they're busy, too, so designing a process that involves IT can slow you down unnecessarily. The smarter choice is a platform that is accessible and user friendly, letting you pull your own reports now, rather than submitting a ticket to IT, and hoping to hear back sometime in the next 3-5 days, pending availability.



Make data-driven decisions

Any screening assay – and, in particular, secondary screening – should be funnel shaped. An entire class of compounds from your library enters the screen, some percentage of those compounds meet the primary endpoint of the screen, and... that's where some screening plans have to stop, recalculate, and start all over with a new endpoint. It's at these decision points in the screening process that many once-funnel-shaped funnels turn into cylinders, when a few compounds or conditions that "almost passed" or "practically passed" are folded into the next stage of screening. It's human nature, but it's most certainly not data driven.

Rather than having to stop, analyze, and redirect your screen, what if you could confidently enable your platform to make the go/no go decisions? In many ways, smart platforms make the most data-driven decisions possible, because they're not colored by program needs or milestones achieved. The goal of automation is to remove the human element, which is less about a future of robot scientists, and more about letting data be our guide. This is the essence of data-driven decision making

Of course, it's possible to be data-driven without automation, but it's a slow, painstaking process, requiring a commitment to established data cut offs and a strict avoidance of making excuses for your compounds. To successfully conduct data-driven manual assays, you'll need to determine what data meets acceptance criteria, and what data will fail. You'll need to stick to these values, because they're the only thing keeping your screening assay from being a moving target. In order to most closely approximate an automated screening procedure, you'll want to make your data cut-off decisions at the beginning, before you start noticing trends and sparse spots. This isn't about ignoring data, but rather it's about impartiality and data integrity.

If you've gotten this far, it probably means that you're interested in achieving the best, most reproducible, and least decontextualized data possible. We hope our common-sense recommendations help you to take the first steps towards a data management plan of your own. If, however, you're in need of something a bit more tangible, you may want to consider investing in a liquid handling workstation. With a flexible automation platform, like Beckman Coulter's Biomek Liquid Handling workstations, managing both your screen and screening data – from sample prep to lead advancement – can be straightforward and traceable, even without help from your IT department. Biomek offers flexible automation for all of your screening successes!

However you choose to manage your data, the most important things to remember are to plan ahead and stick to the plan. For more tips on how to manage your screening data, check out info.beckmancoulter.com/optimize