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AsedaSciences®

The annual listing of 10 companies that are at the forefront of providing Pharma and Life Sciences solutions and transforming businesses

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AsedaSciences®

Combining Data Quality and AI to Transform Drug Discovery

Drug discovery plays a vital role in improving human health, with the pharmaceutical industry focused on maximizing productivity while maintaining patient safety. However, decades of failed clinical trials, a significant proportion of whose root cause stems from animal testing being an imperfect proxy for human safety risk, have reduced productivity. The resulting downstream clinical failures in new molecule development have cost the industry billions of dollars and drives higher drug prices. To address this problem, drug developers have tried to leverage big data to help them identify risky molecule attributes before development. However, a lack of high-quality data is hindering well-informed, data-driven decisions to help save the industry significant resources in its drug discovery journey. How can pharma firms reduce drug screening risks, implement "fail fast" approaches and optimally eliminate late-stage hurdles?

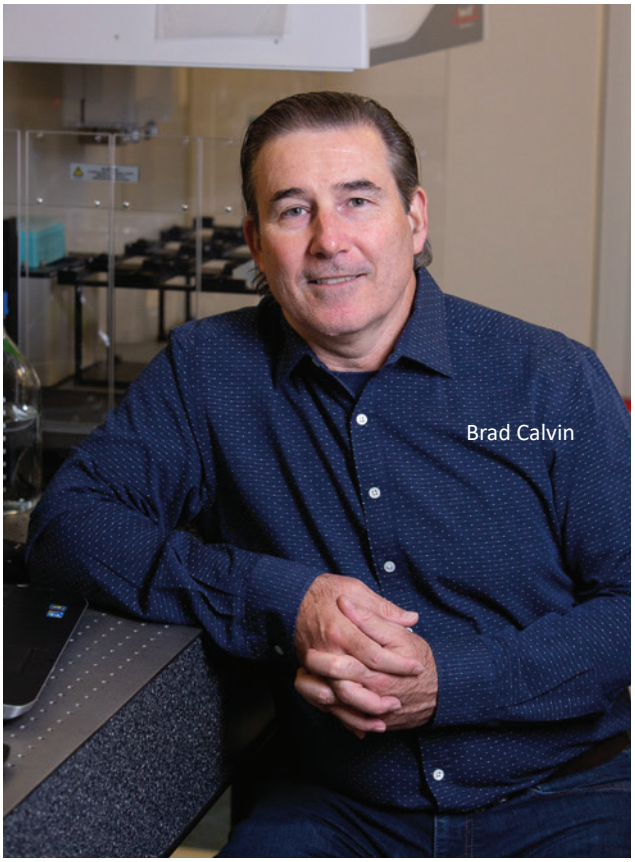
Indiana-based AsedaSciences provides an answer with its optimized safety de-risking and discovery platform that assists compound prioritization in early discovery, helping to triage and progress safer compounds. By integrating reproducible, information-rich live cell flow cytometry screening, with automation and state-of-the-art machine learning (ML) analytics, clients can make more informed decisions on compound design far earlier to improve pipeline prioritization. The company offers multi-parametric, high-content and -throughput phenotypic screening during which an ML classifier estimates compound toxicity risk relative to a carefully custom-built database of thousands of screened compounds, including failed and on-market drugs and research compounds. "We addressed the data reproducibility issues suffered by many similar cell-based screening approaches, which is critical to enabling accurate machine learning-driven predictions. The result is a next-generation toxicity risk assessment that provides medicinal chemists with a sophisticated, yet intuitive design tool that they can use to rapidly design and progress safer compounds. This helps to address industry productivity and ultimately provide for reduced patient risk," says Brad Calvin, co-founder and President of AsedaSciences.

AsedaSciences' platform generates a molecule's biological fingerprint, in the form of a feature vector describing multiple cell stress parameters, and compares this with the feature vectors of previously withdrawn and discontinued drugs, from its substantial library of screened compounds, using proprietary ML algorithms. "Similar to

Unlike live-cell assays that may struggle to provide reproducible results, our platform delivers next-gen drug screens, integrating machine learning to produce high quality, predictive bio-fingerprint data to help medicinal chemists design safer drugs

facial recognition, our platform measures certain phenotypic features of a molecule and compares those with all known undesirable phenotypes to find if there are similarities that signal problems further down the compound's development," explains Calvin. As a result, downstream failure and associated costs can be reduced due to their clients' advanced understanding of their molecule and its risk estimation before starting R&D.

Calvin attributes the proven success of the company's platform to its unique systems-based approach of delivering information of high quality, content, and value from multi-parametric cellular analyses. "For us, it is less about Big Data and more about high-quality data of sufficient quantity to deliver the potential of machine learning", says Calvin. He also stresses how collaboration between AsedaSciences' biologists and computer scientists ensures the platform's sophisticated data generation pipeline and ML algorithms align harmoniously to generate reproducible drug screening results. The teams' expertise, including Calvin's long journey in regulated diagnostics, also played a vital role in ensuring the platform was focused on quality data generation from the start. "Accuracy, reproducibility, and quality are built into our platform at such a scale that our clients can use it to screen thousands of drug molecules over time and connect their internally validated toxicity data to create their own expansive reference set for the future," states Calvin. "Most companies lack the longitudinal and vertical integration of large numbers of compounds and associated biological data of high quality that can allow them to build their own knowledge system. This limits their ability to use the lessons of historical failures to improve drug design and increase productivity gains for the future. AsedaSciences helps address this gap."


Brad Calvin

AsedaSciences' platform also screens chemicals for the agricultural/industrial chemical industry and compares them to its growing library of compounds in this field. Government regulations mandating alternatives to animal testing have forced other segments of the chemical industry to adopt in-vitro testing. "Our ML training set helps reduce agricultural and industrial chemists' reliance on animal testing and provides them with a New Approach Methodology (NAM) that can be more efficient and accurate relative to human toxicity risk," adds Calvin.

Looking ahead, AsedaSciences intends to fulfill its mission to provide chemists with a tool for easier prioritization of safer compounds by launching the SaaS version of its platform. The cloud-based platform, called 3RnD®, will enable chemists to access output from the company's ML algorithms, visualization tools, and an ever-growing library of reference compounds from their own screening database and consolidate all the data in one secure, single pane of glass. "We are not a data storage business but an information generation company, and with our platform's ability to link chemical structure with high-quality datasets, AsedaSciences will continue helping the industry to optimize drug discovery with data-driven precision," concludes Calvin. CR