



3DEXPERIENCE®

STREAMLINING SMALL MOLECULE R&D WITH BIOVIA PIPELINE PILOT STRATEGIES TO MODERNIZE COMBINATORIAL CHEMISTRY

Use Case



Challenge:

Technological and operational complexities in managing an enterprise small molecule combinatorial library made selecting new drug leads slow and prohibitively expensive

Solution:

BIOVIA Pipeline Pilot to automate screening of compound libraries for candidate selection

Results:

- Automated and enhanced input processes for determining chemical compounds
- Increased compound library by 55% while reducing overall operating costs by over 50%
- Efficient and effective access to chemical compound screening

CUSTOMER: A GLOBAL PHARMACEUTICAL PRODUCER

This BIOVIA customer is one of the world's largest pharmaceutical producers, touting a diverse global network of research groups and manufacturing sites. Their aim as an organization is to research, develop and manufacture a diverse pipeline of pharmaceuticals, vaccines and consumer healthcare products. They continually lead the pack in adopting new approaches to improve their R&D capabilities, increasing their R&D productivity and efficiency and supporting their mission to take on some of the most complex problems in medicinal chemistry.

CHALLENGE: EFFICIENTLY SELECTING NEW LEAD COMPOUNDS

The space of drug-like molecules is vast, and determining which to use as a jumping off point for a new lead compound remains a key challenge for medicinal chemists across the life science industry. These candidates must satisfy a number of key parameters, from size to synthesizability to safety. Combinatorial chemistry has allowed pharmaceutical companies to create virtual libraries of related compounds, helping researchers to narrow their focus on those which best suit their needs. Previously, this BIOVIA customer had devoted a large team of medicinal and computational chemists to oversee their combinatorial library, which contained tens of thousands of unique entities. This library needed to be updated frequently to capture the latest regulatory and R&D strategy changes. As a result, the management team would need to assess the millions of compounds available from their various suppliers and filter them down to match the customer's desired specifications. To ensure candidate compounds met researcher's needs, the customer maintained a highly-selective, three-phase process for potential purchase of new compounds. Their efforts focused on screening candidates via a variety of business goals (i.e. cost) and specific physicochemical descriptors. This process was repeated annually.

However, keeping the appropriate balance between these business and scientific goals often resulted screens needing to be run multiple times. These failed runs thus led to increased pressure to meet deadlines and cost efficiency, driving down productivity and increasing the risk for errors in analysis. As a result, managing the library was costing this customer tens of millions of dollars per year. To address this issue, company leadership decided to explore methods to automate the labor-intensive, non-value added steps of the process to streamline compound selection for the library.

"We wrote screening templates and tools within [BIOVIA Pipeline Pilot]. This is the most cost-effective tool I've ever had... It completely saved our sanity."

— Director of R&D,
Global Pharmaceutical Producer

SOLUTION: PIPELINE PILOT TO AUTOMATE CANDIDATE SCREENING

For the customer's high-throughput screening processes, BIOVIA Pipeline Pilot compartmentalizes their data on their extensive variety of chemical compounds and controlled substances. This has helped alleviate any foreseeable issues with legislative shifts and allotted for a pharmacophoric approach to candidate selection. Pipeline Pilot allows this customer to meet their goals of archiving compound collections based on a variety of parameters, including desired physicochemical properties, molecule complexity, and synthesis cost, among others.

By developing a mathematical model within BIOVIA Pipeline Pilot that parameterized historical screening data, the customer was able to determine—based on a particular portfolio of targets and possible compounds—which compound in their extensive library would give the maximum return. They are able to manage their supply chain of external companies with greater ease. Through filters and caches created in Pipeline Pilot, the team has removed mistakes in their acquisition processes and compound collection protocols. By alleviating the often painstaking difficulties involved in these processes, they have stemmed employee turnover and streamlined processes. This, according to one team member, has "completely saved their sanity."

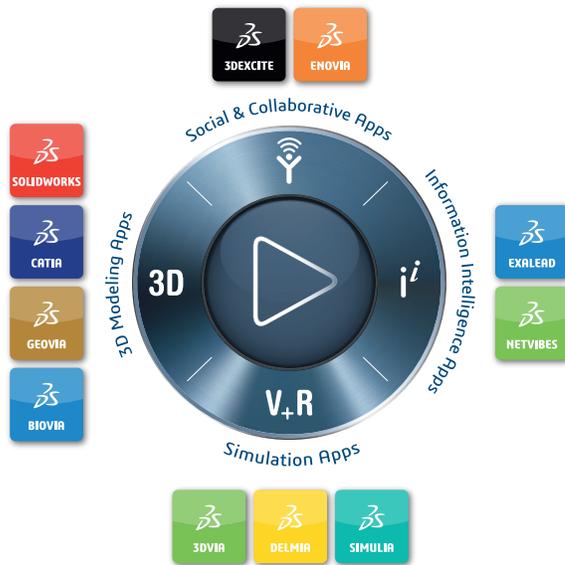
RESULT: A STREAMLINED PROCESS FOR COMBINATORIAL CHEMISTRY

BIOVIA Pipeline Pilot has helped the customer create effective protocols to streamline their chemical compound collection processes. In addition to reducing overall operational costs, they were able to overcome many bottlenecks in their automation facilities, eventually changing the scope of their processes

entirely. They were not only able to increase their compound library by 55% with these transitional changes in place; they also reduced costs to maintain this increased library by more than 50%. The team that works today at this BIOVIA customer now has efficient and effective access to high-throughput screening data, along with automated and enhanced input process for determining chemical compound collection. This has led to improved synchronization and continued vetting of their compound collection processes.

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