BIOVIA

3DEXPERIENCE®

SMALL MOLECULE THERAPEUTICS DESIGN

TRANSFORMING DRUG DISCOVERY THROUGH AI-DRIVEN ACTIVE LEARNING

Datasheet

DASSAULT SYSTEMES

On average, it takes 12-14 years and $2.6B dollars to develop and launch a new drug. The first step to this is the drug discovery phase. It typically takes around four years and in the case of small molecule therapeutics, requires over 4,000 compounds to be synthesized and screened. To significantly accelerate the innovation cycle, advance drug candidates to the clinical phase more rapidly and increase competitiveness, organizations require a transformational approach in drug discovery. They need to:

- Develop innovative new therapeutics for novel diseases more rapidly
- Minimize experimental cost and timelines
- Reduce the failure rate of drug candidates in the clinical phases

INTEGRATED DRUG DISCOVERY WORKFLOW

Drug Discovery transformation requires an integrated drug discovery workflow that combines both *in silico* and experimental approaches (or the 'Virtual' and the 'Real' ('V+R')). BIOVIA has created a dedicated, integrated solution for Small Molecule Therapeutics Design that includes all capabilities for V and R relevant to a modern discovery organization. It includes capabilities to design and perform physical lab experiments, to record results obtained and to register the molecules in a seamless and efficient way. This increases lab productivity and shortens the R-cycles. Adding *in silico* methods such as molecular modeling and machine learning (ML) will provide the needed insight into intermolecular mechanisms. Artificial Intelligence (AI) helps scientists to generate ideas for compounds to synthesize next that get them closer to a desired target product profile taking into account activity, anti-target effect, ADME and toxicology profiles. Sharing validated models to the entire discovery team extends the reach of modeling experts. The V-cycle - the automated virtual creation, testing and selection of novel small molecules - helps design and develop drug candidates with optimal efficacy and safety profiles and at lower cost. In order to establish AI-driven Drug Design as a practice within a discovery organization it is essential that all aspects of this process and all people involved are using applications that are fully integrated and built on a common informatics backbone.

Accelerate drug discovery workflows and reduce time-to-market by designing small molecule drug candidates with optimal efficacy and safety profiles.

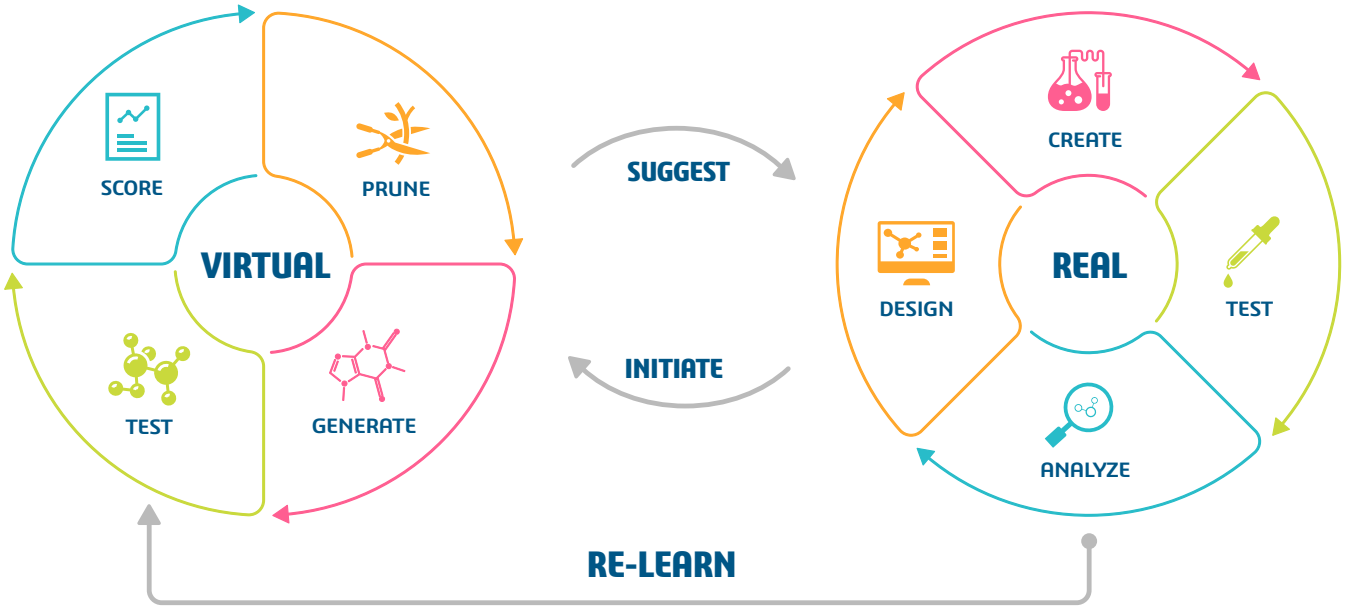

Figure 1. By combining physical testing in the lab (real) with *in silico* (virtual) in an iterative way, organizations can speed the drug discovery process by as much as 50%, by 1) reducing the number of active learning cycles and 2) shortening the time for each active learning cycle.

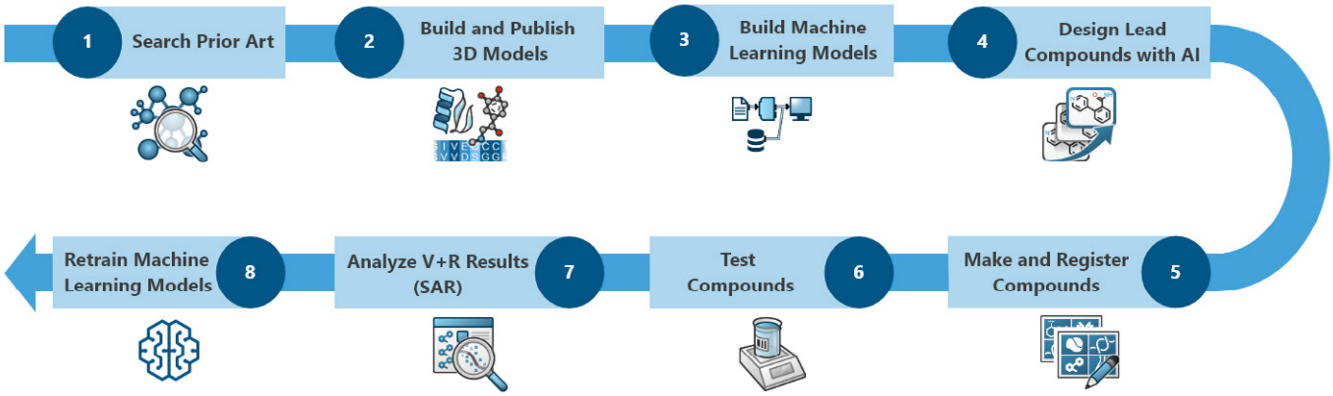

Figure 2. The Small Molecule Therapeutics Design workflow involves a series of activities done in various applications to manage the V+R active learning process

The Virtual

By leveraging *in-silico* capabilities, BIOVIA's solution for Small Molecule Therapeutics Design adds an additional dimension to Drug Discovery by allowing scientists to virtually identify and optimize therapeutic small molecules before, and in addition to physical testing.

AI allows medicinal chemists to quickly generate ideas for compounds to make next in order to get closer to their target product profile. They can apply ML models and physics-based methods built and configured by in-house experts without having to learn how to build them. This approach helps to reduce the number of physical experiments that are required to find a lead candidate. It also helps scientists to increase the number of leads and to identify truly novel, non-obvious molecules through de novo exploration of chemical space.

This process is challenging because it requires multiple properties in a Target Product Profile (TPP) to be optimized simultaneously. A multi-objective optimization algorithm will balance properties such as on-target activity, off-target selectivity, ADME, safety and toxicity profiles, developability and even ease of synthesis, to develop new molecules that have an increased chance of meeting the TPP.

Methods that are particularly valuable in the generative design process are pharmacophore scoring and docking simulations. Even though these techniques can be rather expensive, running them in a scalable cloud architecture makes it possible to apply these to very large virtual chemistry data sets. These 3D methods are essential for generating high quality molecules.

Molecular modeling and simulation techniques allow computational chemists to support chemists doing designs by building and publishing highly accurate models built for their specific targets of interest. These models can be managed and life-cycled in the cloud, and requires no involvement from IT or software developers.

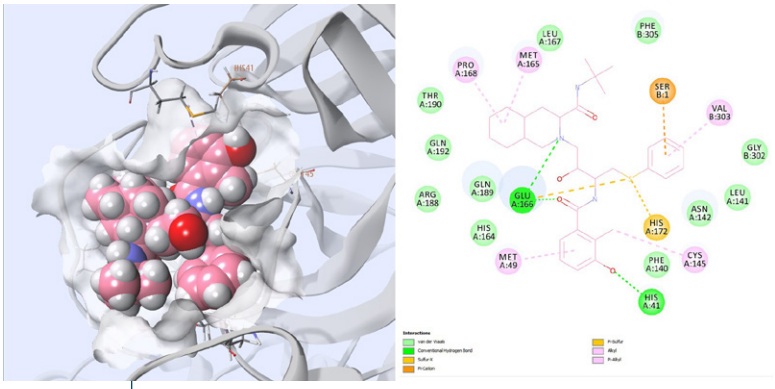

Figure 3. (left) A candidate drug docked in a protein's binding pocket; (right) a map of the intermolecular interactions between the protein and ligand.

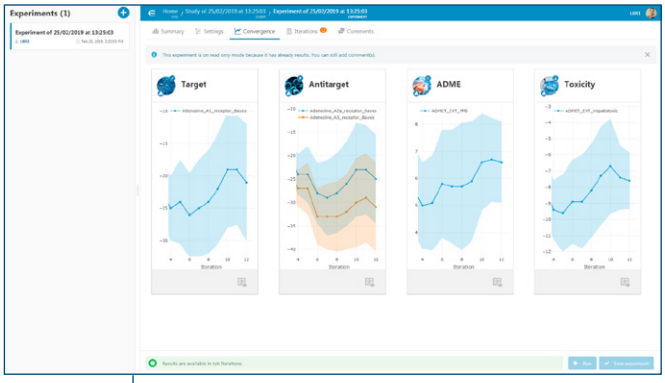

Figure 4. The system helps you monitor the progress of the multi-objective optimization process, as it is balancing multiple properties that are often competing.

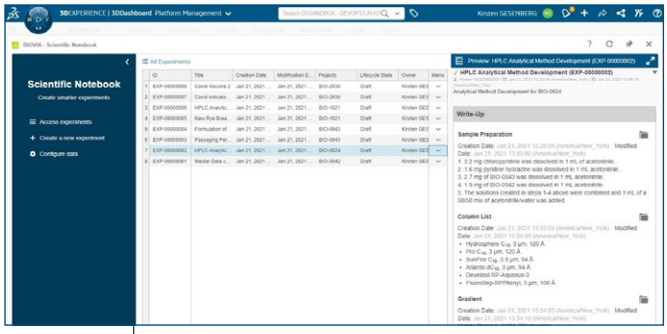

Figure 5. A cloud-based electronic lab notebook helps scientists to design, plan, record and analyze experiments, draw conclusions and document the outcome. Automated capturing of results, signatures and countersignatures ensure IP protection.

Using the automated virtual creation and testing of novel small molecules will optimize lead molecule design in advance of physical testing. This makes physical testing more targeted, reducing drug discovery cycle times and costs.

The Real

BIOVIA's solution for Small Molecule Therapeutics Design supports scientists' workflows in the lab end-to-end. They can efficiently design, plan, record and analyze physical experiments, draw conclusions and document outcomes through an intuitive user interface. It supports and documents the creation, management and consumption of samples and lab materials ensuring real-time inventory overview. The integration of compound registration, data capture and analytics, experiment authoring and review ensure the secure capture of valuable data, documentation and scientific expert knowledge. This allows its reuse across projects and within R&D communities and protects intellectual property (IP). Team members can unambiguously identify chemical and biological substances and share the data within and across teams. A team of scientists can collaborate and contribute to the same experiment in real-time. Overall, it speeds physical lab experimentation and supports collaboration and knowledge management.

Producing Safer, More Efficacious Therapeutics Faster

BIOVIA provides an integrated, robust and agile solution for Small Molecule Therapeutics Design that combines virtual and real activities in a collaborative cloud environment. The synergy between *in silico* methods for virtual identification and optimization of compounds and physical experimentation at the bench drastically improves R&D productivity, helping teams deliver safer, more efficacious treatments to patients faster than ever before.

With the BIOVIA solution for Small Molecule Therapeutics Design, drug discovery teams can:

- Collaboratively design lead candidates in a single integrated environment
- Reduce physical experimentation with validated predictive models and *in silico* experiments
- Increase number and quality of lead therapeutic candidates with improved safety profiles
- Increase success rate by designing molecules with desired properties
- Democratize high-quality, up-to-date predictive models

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