BIOVIA QSAR WORKBENCH

DATASHEET

In the past 15 years, automation in drug discovery projects led to massive increases in the amounts of data generated by multifunctional chemistry and biology teams. Data trends and patterns can help project teams make important decisions about what entity to make next in a series. The challenge is how to speed the process and reduce costs.

Developed in collaboration with pharmaceutical company GlaxoSmithKline, the BIOVIA QSAR Workbench automates and accelerates the development, validation, deployment and life cycle management of predictive Quantitative Structure-Activity Relationship (QSAR) models. Built on the BIOVIA Foundation, the QSAR Workbench utilizes native QSAR methods in Pipeline Pilot and easily integrates with other statistical tools. Each step in QSAR model development is encapsulated in discrete Pipeline Pilot protocols, ensuring that the best practices of the statistical experts are accurately captured and repeatable.

REDUCE QSAR MODELING TIME FROM DAYS TO HOURS

It typically takes an expert statistician 5 to 10 days to deliver a new predictive QSAR model. Multiple software packages—each with its own user interface—are often used to prepare and calculate molecular descriptors, and then build and validate each QSAR model. This process is manual, tedious and prone to errors.

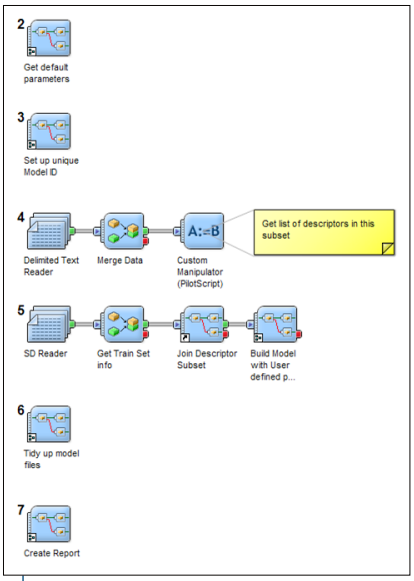

Figure 1: Easily extend the range of statistical methods available utilizing the underlying Pipeline Pilot technology.

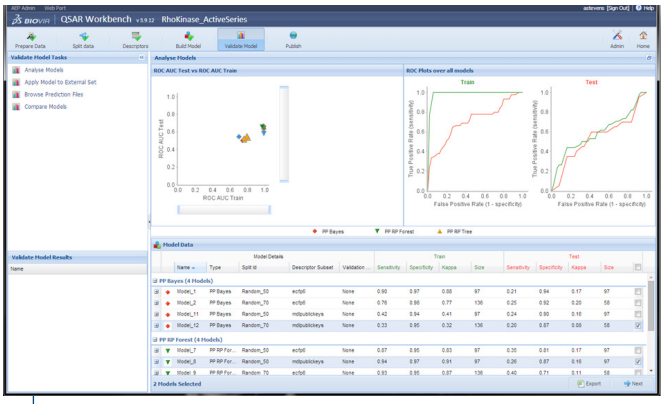

Figure 2: Rapidly explore and compare statistical space to identify robust, predictive QSAR models.

The QSAR Workbench dramatically simplifies and streamlines model development from days to hours, providing a single guided interface that enables dataset management, descriptors selection , and selection of statistical modeling and validation methods. It provides the ability to record, play, and re-play modeling building workflows, meaning that new screening data can be run in a matter of minutes by the original methods developer or another scientist.

The QSAR Workbench enables experts and non-experts alike to save time, reduce costs, collaborate more effectively and speed research by leveraging robust, predictive models.

EXTEND THE REACH OF STATISTICAL EXPERTS

Once the models are created by the QSAR experts they can be easily published directly to the chemists on project teams, using applications such as BIOVIA Insight, who can test their hypotheses *in silico*. This enables the statistician to focus on delivering models and empowers the chemists to execute their models on their datasets. This saves time and reduces costs. The model life cycle management capabilities helps the computational experts ensure the chemists are always using valid up to date models.

WHAT QSAR WORKBENCH DOES

- Enables statistical experts to capture QSAR model development best practices
- Enables both QSAR experts and other scientists to fully explore all combinations of molecular descriptors, QSAR models and parameters
- Automates model development processes through its ability to record and playback multiple steps in sequence from a QSAR study
- Keeps QSAR models up-to-date as new assay results become available and manages the life cycle of the models
- Uses Pipeline Pilot technology to expose and automate Pipeline Pilot QSAR methods such as Bayesian, Recursive Partitioning, Neural Networks, and Linear Regression
- Allows validated models to be published directly to end users using other application such as BIOVIA Insight
- Enables third-party molecular descriptors and statistical methods to be integrated using Pipeline Pilot

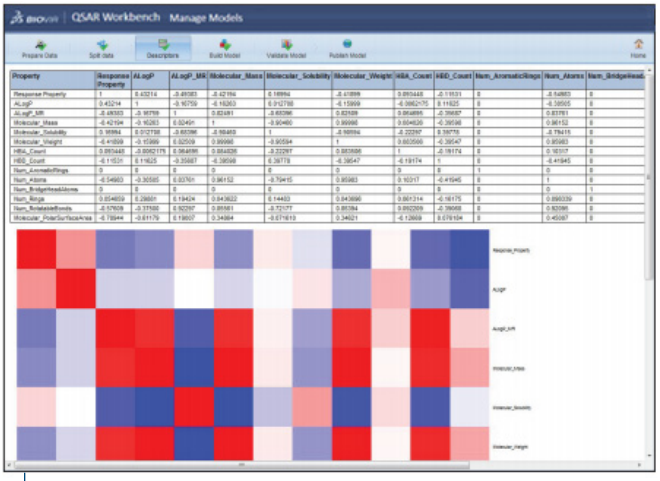

Figure 3: Quickly visualize relationships between molecular descriptors and biological endpoints.

WHO BENEFITS

- **Computational Chemists:** Capture best practices and automate the tedious, error-prone steps of model building. Facilitate collaboration with project teams to speed decision making and ensure model validity.
- **Medicinal Chemists:** Access the latest project QSAR models to test more hypotheses *in silico*—resulting in faster, better decisions.
- **Research Managers:** Enable your statistical experts to easily share their expertise and collaborate with your entire computational team—speeding research, making more informed decisions and reducing cost.

EXAMPLE TASKS

- **Split data set:** Specify training and test data sets using a variety of methods, e.g. random percent, by chemistry or property cluster or even interactively
- **Calculate descriptors:** Utilize hundreds of different 1D, 2D and 3D molecular descriptors leveraging Pipeline Pilot's native chemistry calculators or integrate with third-party calculators
- **Build multiple models:** Derive multiple QSAR models, explore different descriptor sets, statistical methods, their associated parameter sets and even data splits
- **Compare multiple models:** Directly compare the statistics and test set results to identify the optimal predictive models for each statistical method
- **Publish models and methods:** Save and publish optimal models and new methods so they can be immediately used by others

To learn more about QSAR Workbench, go to
accelrys.com/products/qsar-workbench.html

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