BIO-RAD

Integrated Tools for
ADME/Tox Prediction

www.knowitall.com

BIO-RAD

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Minimum System Requirements: Windows-compatible PC, CD-ROM Drive, Windows 2000, Windows XP Home, or Windows XP Professional operating systems, Pentium III (or equivalent) processor, 128 MB of RAM, 100 MB of free hard disk space (Additional disk space required for HaveItAll® databases.)

96210

KnowItAll®
Informatics System

KnowItAll is the Power of Integration

Chemists and biologists continue to face increasing pressure to evaluate compounds quickly and identify candidate failures early.

Bio-Rad's award-winning KnowItAll® Informatics System puts tools at the fingertips of the researcher to assess the ADME/Tox profile of potential lead compounds in the initial phases of drug discovery. KnowItAll offers a complete and fully integrated software environment for ADME/Tox prediction, the world's largest collection of predictors, and tools for structure drawing, database management, and customized reporting. The result is a shortened research-to-market cycle and the elimination of wasted R&D effort.

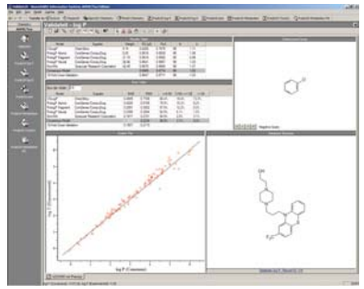
Drug Candidate Design

Individual structures or databases of structures

In Silico Prediction of Properties

Candidates can be screened for multiple properties

Validate & Predict



Bio-Rad Offers the World's Largest—and Fastest Growing—Collection of ADME/Tox Property Predictors.

- Absorption Rate
- Bioaccumulation
- Bioavailability
- Blood-Brain Barrier Permeability
- Elimination Half-Life
- First-Pass Metabolism
- Immunotoxicity
- Irritation
- log D
- log P
- Metabolism
- Metabolite Toxicity
- Mutagenicity
- Neurotoxicity
- Oncogenicity
- Plasma Protein Binding
- pK_a
- Polar Surface Area
- "Rule of Five" Violations
- Sensitivity
- Teratogenicity
- Volume of Distribution
- Water Solubility
- And More

Contact Bio-Rad for an up-to-date listing of prediction models.

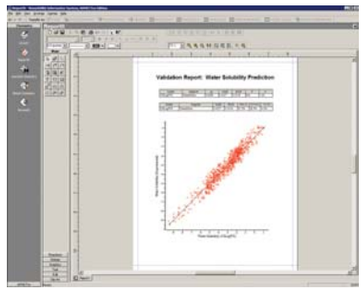
Consensus Modeling for Accurate Predictions
With Bio-Rad's KnowItAll Informatics System, multiple predictive models can be combined as a single consensus model to achieve the most accurate predictions. The system can be trained for optimal results in a current project and later retrained for other projects. As a result, the researcher can produce results that are superior to any single model. Predictably.

Validation of Predicted Results
For all property prediction types, whether a consensus model or single model is used, the KnowItAll ValidateIt application provides statistical validation of the prediction model by comparing experimental results to predicted results. The statistical analysis includes error binning, scatter plotting, mean absolute error, root mean square error, N-fold cross validation, and other tools for validation analysis.

Evaluation of Screening Results

Data are compiled and saved for review and data mining

Report



Accelerate Lead Generation with:

- The largest collection of prediction models
- Multiple models for more accurate predictions
- Powerful validation tools to verify models
- Integrated toolset for improved workflow

Successful Candidates

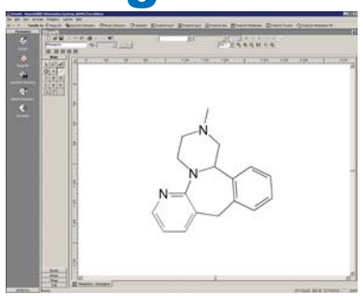
Continue with subsequent testing and evaluation

Iterative Re-Design

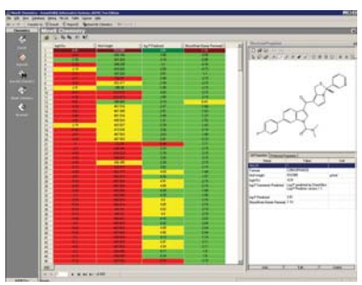
Structures can be modified and re-screened

Design

Integrated Structure Drawing
KnowItAll includes DrawIt™, a fully integrated, feature-rich, structure drawing tool (developed using Bio-Rad's well-known ChemWindow software). With DrawIt, regardless of how the structures were drawn originally, they can be modified and immediately re-evaluated without the inconvenience of transferring information to and from external software.



Analyze



Integrated Toolsets for Improved Workflow
KnowItAll integrates its comprehensive collection of ADME/Tox predictors into a single unified environment that also includes functionality for structure drawing, analytical informatics (NMR, LC/MS, IR, and Raman), data mining, building and maintaining databases, and reporting.

To improve workflow, all of these tools are provided in one consistent interface for seamless import and transfer of data from application to application.

The result is a system that handles all of your *in silico* ADME/Tox prediction requirements in a single application—with more accurate results, including complete statistical validation—all in an environment that allows you to close the loop on structure design, prediction, analysis, results management, and reporting.