

Desktop decision support for scientific research

Visualize and analyze diverse chemical and biological data

Easy to use histograms, graphs, color coding, R-group analysis and recursive partitioning make it simple to interpret your data

Cheminformatics Datasheet

DIVA

Getting the most from large amounts of chemical and biological data is a key challenge for today's researchers. Accelrys has designed DIVA to handle that challenge, giving you the tools you need to work with your chemical and biological data.

Maximize the value of your chemical and biological data

DIVA provides a complete, integrated set of decision support tools on your desktop, helping you to carry out tasks faster and more efficiently.

DIVA delivers power to your desktop, letting you gain more value and deeper insights from your data investment. DIVA also improves communication, facilitating the sharing of information through powerful reporting tools.

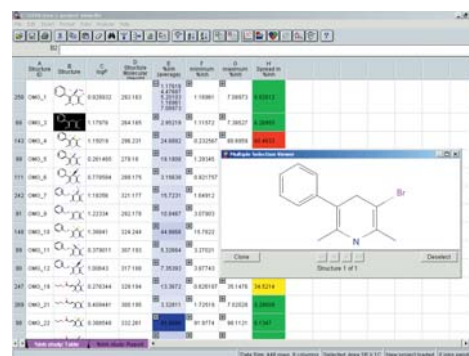
Support for every step of data analysis

Researchers want to spend their time evaluating promising compounds, not unraveling experimental results. DIVA's interlinked tools facilitate that goal, helping to:

- Locate valuable results and read files with chemical and biological data, regardless of location or point of origin.
- Assemble and organize those results in meaningful ways for analysis, including automatic merging and rearrangement.
- Visualize those results, to spot trends, patterns and anomalies, using interactive graphical tools.
- Analyze and extract maximum value from that data to guide your next research steps.
- Communicate and share those results, findings and suggestions via forms-based reports.

Find your data regardless of location

DIVA readily works with all data types – structures, compound identifiers, numerical and text – and holds them in one convenient project format with a familiar spreadsheet view. To further improve efficiency, DIVA consolidates information on compounds from disparate sources to create merged reports and spreadsheets.



▲ DIVA integrates chemical and biological assay data, searchable by structure or substructure

Assemble data from many sources

Combining data from multiple sources into a single, uniform data set that is ready for analysis is a simple task with DIVA. The tools in DIVA allow for simple merging and pivoting of rows and columns, allowing commonly needed transformations of assay results and other experimental values to be performed in seconds. Simple applications include: row merging, column pivoting, column merging, summarizing multiple value cells, and splitting into rows.

Organize information to best communicate results

With DIVA, data can be organized using colors – in the most intuitive ways – flagging and grouping results to share with other team members. For example, chemically similar functional groups or classes can be grouped, while ADME screen data can be flagged as acceptable, unacceptable or cautionary.

Quickly identify patterns and trends

DIVA incorporates a wide range of visualization techniques that enable scientists to look at their data from multiple perspectives. Those techniques have been selected and developed in collaboration with researchers to help them better tackle research projects. For example, alignment by common substructure or identification of characteristics such as molecular weight can be used to highlight items of interest for subsequent analysis.



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Identify important relationships with graphs

2D or 3D graphs can be built using a number of data variables. Color-coding can be added to create a 4D representation of a data set. DIVA gives the user full control over the graph display, including rotations and transformations. Multiple graphs can be on-screen at the same time, allowing alternative views of the same data to be compared.

Recognize structure variations in combinatorial libraries

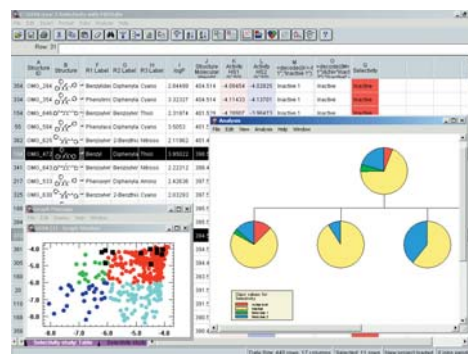
When working with a set of compounds with a common chemical core, as found in many combinatorial libraries, DIVA can automatically locate and name the variable substituents for every compound in the set. This simple process lets scientists easily see the variation in structure to compare compounds visually. Plus, the R-group names are perfect descriptors for use with histograms or FIRM analysis, enabling quantitative assessments of how variation in structure affects activity.

Correlate data to drive your next research steps

When many columns of data are available, such as test results for a set of compounds across many different assays, it is important to see how they interrelate. DIVA's histograms allow a researcher to compare how compounds perform in different experiments – for example, to detect trends in selectivity – while correlation analysis gives a visual display of how overall results for different assays are related.

Categorize and analyze data using statistics

FIRM (Formal Inference-based Recursive Modeling) is a powerful decision tree analysis tool that can be easily used to analyze and explain data. FIRM automatically finds the mathematical rules that explain your data and displays the results in an intuitive graphical form. The results quickly highlight important trends and patterns that can lead you to real insights. Because FIRM is automatic and uses robust algorithms, you don't need to be an expert statistician to benefit from its power.



▲ *Graphs and recursive partitioning analysis give you an instant insight into your data*

Create your own reports

The powerful and flexible forms-based report generator in DIVA enable each user to create report formats that show the selected data set in the exact format desired. The user can choose the information – including multiple chemical structures within a single cell – the labeling and positioning of that data, and copy/paste it into common desktop programs. Plus, graphical displays and accompanying data can be stored in a project file and shared with colleagues.

Gain full value from Oracle® with RS³ Discovery

The desktop version of DIVA gives scientists a powerful decision support system for integrating and analyzing biological and chemical data. DIVA can also connect directly to your chemical and biological Oracle databases using Accelrys' RS³ Discovery™ and Diamond Discovery™ servers.



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