



Benchware

Pantheon for Users

Organize, analyze, and visualize chemical and biological data



FEATURES

- Intuitive and easy to use for any scientist
- Data organization tools
- Chemically aware spreadsheet
- 2D chemical structure grid viewing
- 3D chemical model visualization
- Rich set of chemical descriptors
- Hook to any data source: no external database required
- Integrated with industry standard chemistry tools (e.g. ChemDraw and SymyxDraw sketchers)

Benchware® Pantheon™ is an affordable, extensible cheminformatics solution that enables discovery scientists to organize, analyze, and visualize chemical and biological data and make better decisions faster.

How much time have you spent cutting and pasting data from one spreadsheet to another just to get all your data together in one place? With Pantheon, merging data from multiple sources and types is as easy as dragging and dropping.

Need to merge biological data with chemical structures? No problem. Multiple file formats? Excel? SDF? Smiles? Mol2? No problem. Pantheon automatically handles translations from a range of industry standard formats so you don't have to think about it.

And once you have your data together, Pantheon provides a rich set of capabilities for formatting, sorting, filtering, analyzing and visualizing your data. Because Pantheon is "chemically aware," Pantheon understands the chemical structure in your spreadsheet and can quickly calculate a wide range of molecular properties.

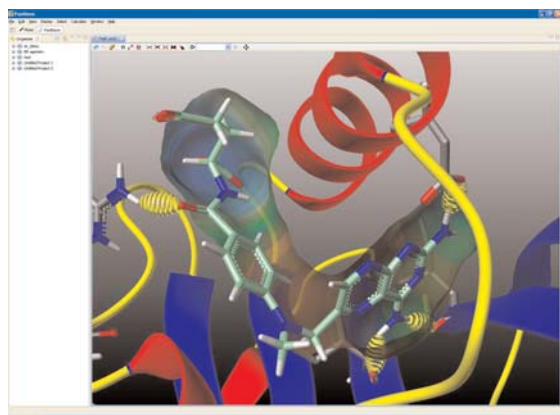
The screenshot displays the Pantheon application window. On the left is a file organizer tree. The main area shows a spreadsheet with columns for 'Molecule', 'EXTREG', 'Date synth.', 'FA', and 'Date tested'. Several rows contain chemical structures and associated data. A 'Merge by Match' dialog box is open, showing a table of records to be merged. The table has columns for 'Molecule', 'EXTREG', 'Date synthesized', 'FA', and 'Legend'. The records are as follows:

Molecule	EXTREG	Date synthesized	FA	Legend
AP-0002	11/2/2008	1.2	0	Empty or untouched cell
AP-0002	2/23/2009	3.4	0	Empty or untouched cell
AP-0005	3/11/2008	3.4	0	Empty or untouched cell
AP-0005	4/02/2008	4.5	0	Empty or untouched cell
AP-0005	1/13/2008	9.08	0	Empty or untouched cell
AP-0006	6/21/2008	7.8	0	Empty or untouched cell
AP-0006	7/29/2008	9.1	0	Empty or untouched cell
AP-0009	9/30/2008	9.8	0	Empty or untouched cell
AP-0011	11/17/2008	9.8	0	Empty or untouched cell
AP-0012	12/11/2008	3.41	0	Empty or untouched cell
ZETA23		9.08	0	Empty or untouched cell
ZETA24		4.95	0	Empty or untouched cell
ZETA99		9.11	0	Empty or untouched cell
ZETA81		8.77	0	Empty or untouched cell
ZETA912		9.22	0	Empty or untouched cell

Using Pantheon, scientists have the capabilities to easily merge chemical and biological data from Excel spreadsheets or other disparate data sources.

Pantheon

What makes Pantheon unique is the combination of a chemically aware spreadsheet and "grid view" with powerful 3D molecular visualization. With Pantheon, you can visualize the binding interactions of a drug candidate with its receptor and also view all the biological testing data and molecular properties of the candidate. Pantheon gives you the FULL picture of your data.



Pantheon provides users with crisp, compelling, interactive 3D visualization of molecules

Operating system requirements

Windows XP or Vista

Hardware requirements

32-bit chip only

Complementary software

Benchware® Muse™

Tripos Chemistry Extensions for KNIME™

Need to communicate your results to other team members?

No Problem. Simply e-mail your Pantheon files to a colleague and they will instantly see what you see. Pantheon provides powerful integration with key productivity applications like Microsoft Excel and Powerpoint.

With Pantheon, 3D molecular images embedded in Powerpoint aren't just static "pretty pictures" but fully interactive molecular visualizations that can be rotated, scaled or modified to communicate fully the essence of your discovery.

Problems Pantheon Addresses

- Analyze and visualize biological and chemical data together

Example: Merge assay results sent to you in Excel spreadsheets by multiple biologists with chemical structure information

Example: Analyze a set of lead structures against multiple criteria in your projects biological cascade. Compute molecular properties, perform multi-criteria sorting and filtering to prioritize your project's leads.

- Sharing of Results and Experiments between users

Example: Create a PowerPoint presentation with 3D visualization that highlights key drug-receptor interactions.

Download a free 30-day evaluation in the Free Software section at:

www.tripos.com/download
Registration required