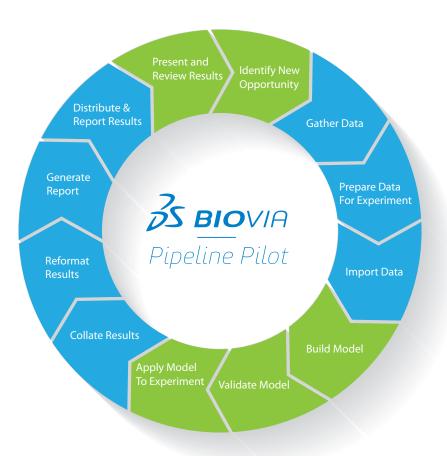




# **PIPELINE PILOT OVERVIEW**

Datasheet



BIOVIA Pipeline Pilot optimizes the research innovation cycle by providing capabilities for scientific analysis (in green) and allowing for the automation and standardization of manual, repetitive data preparation and collation tasks (in blue).

This allows scientists and engineers to spend more time applying their skills and knowledge where innovation takes place.

BIOVIA Pipeline Pilot is a graphical scientific authoring application that optimizes the research innovation process, increases operational efficiency and reduces costs for both research and IT. Pipeline Pilot automates the scientific analysis of data, enabling users across the enterprise to rapidly explore, visualize and report research results.

# WITH PIPELINE PILOT YOU CAN:

- Complete projects significantly faster (10x or more) by leveraging existing research and intellectual property and automating routine data gathering and analysis processes
- Uncover the knowledge hidden in your data by quickly aggregating and processing massive volumes of structured and unstructured data from multiple disparate research areas in a single environment

- Encapsulate and deploy best practices to ensure compliance and enable collaboration across your research and development organizations
- Reduce direct research costs by developing models for discovery based on predictive science
- Rapidly build and deploy high quality scientific solutions based upon standard technologies and widely accepted
- Improve decision making with better, faster experimental results through real-time reporting dashboards

### **POWERFUL DATA PROCESSING**

Pipeline Pilot utilizes a powerful data pipelining engine that executes data processing procedures developed within the Pipeline Pilot graphical authoring environment. By doing this, Pipeline Pilot facilitates the development, standardization, and automation of scientific data management, analysis and reporting.

# "Numerous pre-defined components have helped us to construct applications that would have required months of development with a traditional coding language."

- Computational Scientist, Global 500 Pharmaceuticals Company

# Pipeline Pilot delivers:

- Data management, analysis and reporting for text, numeric and complex scientific data, including chemical structures, biological sequences and scientific images
- A rapid application development environment for engineers, developers and scientists that implements standard software development processes using a graphical design interface
- A large (> 2000) set of "scientific building blocks" components that snap together, allowing rapid creation of all aspects of data processing, including data retrieval, manipulation, computational analysis, filtering, and display
- "Build-your-own" component capability leveraging standard technologies including REST Web Services, Python, Perl and lava
- Validated scientific components and best practice workflows that cover a broad range of scientific disciplines

#### **CAPTURE AND DEPLOYMENT OF BEST PRACTICES**

With Pipeline Pilot you can encapsulate, annotate and version your organization's best practices to document and reproduce the steps used to achieve a particular result. Your resulting Pipeline Pilot protocols can be published and shared with others to facilitate cooperative development and knowledge transfer. To make your automated process available to an even wider community, you can make Pipeline Pilot protocols available via web interfaces, including Pipeline Pilot Web Port, SharePoint, custom clients, and other deployment models.

# CUSTOMIZED REPORTING AND WEB APPLICATION DEVELOPMENT

You can create customized reports that summarize your data analysis and mining protocols with a full range of text, tables, charts and images. As you have complete control over the layout and content, you can easily interpret and communicate your results.

By displaying multiple tables, charts and images in a single report, you can see different views of your data including side-by-side comparisons from different sources and data that was processed in different ways. You can deploy your reports in a wide variety of formats including HTML(5), PDF, Word, Excel and PowerPoint.

To make your reports more dynamic, you can add interactivity, linking within, between and outside reports. You can further extend the interactivity to create web applications that link several protocols together into a functional unit.

# **Extend the Power of BIOVIA Applications**

As well as being a great tool for personal and workgroup productivity, Pipeline Pilot can also be used to extend and enhance other BIOVIA applications, including, but not limited to, Insight, Insight for Excel, Workbook, Notebook and EKB. Most BIOVIA applications have specifically designed extension points whereby Pipeline Pilot protocols can provide computational services, create charts or full reports, be used to load data from files, databases and online resources, and integrate with other applications and instruments. Given the nature of Pipeline Pilot, the possibilities are endless! The end-user of the application is typically unaware that they are running Pipeline Pilot protocols, meaning that those end-users gain the benefits of the broad and deep capabilities of Pipeline Pilot and the component collections while keeping the user interface very simple – either the press of a button or a simple configuration form.



"Pipeline Pilot has made data collection, aggregation, and report preparation incredibly easy by cutting down on processing time as well as time taken to correct human error. In addition, it has also paved the way for standardized report outcomes and helped establish key best practices."

- Data Analyst, Global 500 Pharmaceuticals Company

#### **CLIENTS**

# **Pipeline Pilot Professional Client**

The Pipeline Pilot Professional Client is the authoring tool for creating data pipelining protocols. The Professional Client can be used to create and modify protocols for individual use and also to publish them for others to use. The Professional Client can also be used to create new components, or edit existing ones, to meet the varied needs of an organization.

# Pipeline Pilot Web Port

Pipeline Pilot Web Port is a browser-based environment allowing the power of Pipeline Pilot to be extended to a broad community of users. The same protocols that Pipeline Pilot Professional users create and run can be made accessible to Web Port users, thereby exposing the full capabilities of Pipeline Pilot to a wide audience through a simple web-based interface. Web Port users can browse available protocols and parameterize them to run their own data to suit their unique needs, without having to understand how the protocols were built. Users of Web Port can also access and execute protocols via any other web-based interface, such as Microsoft SharePoint, RSS feeds, web-links, and custom interfaces developed with any of the Pipeline Pilot client SDKs.

# PIPELINE PILOT COMPONENT COLLECTIONS

Professional Client users create and edit Pipeline Pilot protocols using Pipeline Pilot components. These "scientific building blocks" are grouped into collections, by category of science or function. The collections contain numerous components which allow researchers, developers, engineers and IT professionals to perform both science-specific and generic data-processing functions. By graphically combining components, you can construct workflows for data retrieval, filtering, analysis and reporting.

# **CHEMISTRY**

#### Chemistry

Analyze, profile and manage the compounds in your corporate database with chemically intelligent filters and learning. The collection also includes the Chemistry Cartridge - a high performance data cartridge that enables you to store and search chemical structures and reactions in Oracle.

#### **ADMET**

Calculate predicted absorption, distribution, metabolism, excretion and toxicity (ADMET) properties for collections of molecules such as synthesis candidates, vendor libraries and screening collections. The collection includes models for human intestinal absorption, aqueous solubility, blood brain barrier penetration, plasma protein binding, cytochrome P450 2D6 inhibition and hepatotoxicity.

#### **BIOLOGY**

# Gene Expression and Mass Spectrometry

Gene Expression focuses on visualizing, analyzing, annotating and reporting on gene expression experiments including the individual target genes. Core functionality is based on BioConductor—the open source software for the analysis and comprehension of genomic data. Mass Spectrometry offers a comprehensive set of components and example protocols to create and automate customized proteomics and metabolomics workflows.

#### **Sequence Analysis**

Analyze, annotate and compare biological sequences in an environment where modular tools can be graphically linked together to create practical bioinformatics routines.

# **Next Generation Sequencing (NGS)**

Analyze and interpret the massive datasets generated by the most current DNA sequencing instruments. The NGS Collection comes with a comprehensive assortment of NGS data analysis pipelines that are ready to analyze your data with unparalleled power and flexibility.

#### **DATABASE & APPLICATION INTEGRATION**

#### Integration

Part of the base Pipeline Pilot system, Integration enables you to incorporate existing in-house or third-party programs as computational services using Java, Python, REST. Also, retrieve data from Oracle using ODBC and JDBC technologies for analysis or reporting, and store results directly back in your own corporate database.

#### **IMAGING**

# **Imaging**

Imaging delivers capabilities for enhancing, processing, analyzing, integrating, cataloguing, searching and reporting image data. It integrates image data with numerical, chemical, graphical and textual data in a unified computing framework.

### **ANALYSIS & STATISTICS**

### **Analytics and Machine Learning**

Carry out powerful analytics and machine learning with this comprehensive suite of learning and data modeling tools, statistical filters and clustering components optimized for large real-world data sets. Access powerful methods such as fast data clustering, Bayesian learning, principal component analysis, linear regression and partial least squares regression. Advanced modeling methods for Recursive Partitioning (RP), Multi-objective Pareto Optimization and a variety of RP

methods are available in the collection including both single tree and forest of tree learners. Additionally, components are available for statistical methods for data manipulation, clustering, learning, classical and exploratory data analysis. The underlying statistical engine is the widely used public domain R statistics package.

#### **MATERIALS MODELING & SIMULATION**

#### **Materials Studio**

The Materials Studio collection allows you to access Materials Studio's premier modeling capabilities within the Pipeline Pilot data pipelining environment. It allows access to analytical capabilities such as Reflex and Reflex QPA, key functionality of the QSAR Plus package and a utility to integrate scripting applications developed within Materials Studio's scripting API into Pipeline Pilot protocols.

#### Polymer Properties (Synthia)

Polymer Properties provides a method for quickly estimating the properties of bulk, amorphous homopolymers and random copolymers based on repeat unit information, molecular weight and temperature.

#### **REPORTING & VISUALIZATION**

#### Reporting

Part of the base Pipeline Pilot system, Reporting offers a comprehensive set of components to create customized reports that you use to display the results of your data analysis and mining protocols. With complete control of what content you include and how to lay it out, you can create highly effective communication tools to share knowledge with your colleagues.

#### **Dashboards**

Easily build modern, responsive dashboards for any device using Pipeline Pilot's built in HTML5 charting capabilities.

#### **LABORATORY**

# **Lab Analytics**

Access methods to read, write, report, visualize, manipulate and perform calculations on plate data. The collection allows each record on the data pipeline to carry an entire plate and its associated wells, enabling you to perform both plate and well-level operations. The collection also supports access to data generated in your analytical lab, e.g., common data processing

operations such as peak identification, peak integration, line width analysis background detection and removal, interpolation, truncation, scaling and smoothing of spectra, subtraction of spectra, general purpose Fourier transform as well as NMR specific functionality.

#### **DOCUMENT SEARCH & ANALYSIS**

#### **Document & Text**

Through document and online resource searching, characterization and analyses, processing routines can be augmented with new information, and users can perform chemically-intelligent text mining of public and internal documents. Advanced capabilities to edit existing documents allow efficient integration between manual document editing and automated analysis and insertion of content.

# **Clarivate Analytics**

With the Clarivate Analytics Cortellis™ collection, you can significantly simplify the process of keeping up with "data deluge" by directly accessing the extensive life sciences information from the <u>Cortellis databases</u> within Pipeline Pilot protocols and seamlessly integrate this with your internal data. The Cortellis collection was built as part of an ongoing partnership between BIOVIA and Clarivate Analytics and provides access to Cortellis databases including Drug Targets, Compounds, Companies, Clinical Trials and Results, and Patents, amongst others.

#### **MOBILE**

#### Mobile

The Pipeline Pilot Mobile collection is built to provide instantaneous access to data and information. By using the ScienceCloud Tasks app, end-users can access powerful but simple-to-use Pipeline Pilot protocols directly from their iPads or iPhones. You can deploy pre-existing Pipeline Pilot protocols, as "tasks" into the app, typically with no changes to the protocol. Additionally, the Mobile collection provides components for rich input (e.g., audio, GPS location, camera) that fully utilize the touch-enabled environment of iOS devices. You can also use the Mobile collection for mobile-optimized (HTML5-based) charting for a sophisticated end-user experience.

To learn more about Pipeline Pilot, go to accelrys.com/pipeline-pilot

# Our **3D**EXPERIENCE Platform powers our brand applications, serving 12 industries, and provides a rich portfolio of industry solution experiences.

Dassault Systèmes, the **3D**EXPERIENCE Company, provides business and people with virtual universes to imagine sustainable innovations. Its world-leading solutions transform the way products are designed, produced, and supported. Dassault Systèmes' collaborative solutions foster social innovation, expanding possibilities for the virtual world to improve the real world. The group brings value to over 170,000 customers of all sizes in all industries in more than 140 countries. For more information, visit **www.3ds.com**.



**3D**EXPERIENCE



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