

BIOVIA Pipeline Pilot

2016 Training Course Catalog



3DEXPERIENCE®

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SUMMARY

We are proud to offer a variety of courses to meet your organization's needs, ranging from navigation basics to advanced technical courses. Customized courses can be designed to meet your organization's specific needs. For more information on customization, please contact your Account Manager.

Delivery Methods:

- Instructor-Led Training (ILT): Facilitated by an onsite instructor, this training takes place at your location or at a selected Biovia site. Each course has hands-on exercises related to the topic of discussion to be completed by the students. Optional manuals are available.
- Virtual Classroom: Using WebEx, our instructors teach these courses virtually allowing students to attend from their remote location.
- eLearning: Intended as a companion to our Instructor-Led Training or Virtual Classroom offerings, these self-paced, computer-based courses cover various BIOVIA Pipeline Pilot-specific topics.

INSTRUCTOR-LED COURSES

PIPELINE PILOT FUNDAMENTALS

This introductory course is beneficial for users with little or no Pipeline Pilot experience. The course covers many of the out-of-the-box components. Students are taught how to use these components to modify existing protocols or create new ones. All basic concepts necessary to create or manipulate protocols are covered. Upon completion of the workshop, students will be able to modify existing protocols and create custom protocols utilizing Pipeline Pilot's wide range of functionality.

Topics	Details
<ul style="list-style-type: none">• Pipeline Pilot overview• Architecture and interface• Developing a running protocol• Checkpoints and design mode• Component collections and types• Filters: Control of flow• Merge and join• Introduction to PilotScript• Subprotocols• Web Port	<p>Duration: 1 day</p> <p>Method: Onsite, Virtual Classroom, eLearning</p> <p>Level: Beginner</p> <p>Prerequisites: None</p>

REPORTING AND INTERACTIVE REPORTING

This course covers the use of the Pipeline Pilot Reporting Collection. Topics cover the use of the static components, as well as the interactive element components available in the Pipeline Pilot Reporting Collection. Users already familiar with customizing components and developing custom protocols will benefit from this course. On completion of the workshop, students will be able to modify and create reports and input forms for running protocols from a browser utilizing Pipeline Pilot's Reporting Collection.

Topics	Details
<ul style="list-style-type: none">• Reporting data structure and components• Building reports that include:<ul style="list-style-type: none">– Text and image– Tables– Charts– Conditional formatting– Interactivity – tooltips, hyperlinks, etc.• Creating input forms for running protocols from a browser	<p>Duration: 1 Day</p> <p>Method: Onsite, Virtual Classroom, eLearning</p> <p>Level: Intermediate</p> <p>Prerequisites: Fundamentals</p>

ADVANCED PILOTSRIPT

This course teaches students the more advanced features of PilotScripting, which includes working with arrays and using variables and functions in protocols. Upon completion of the workshop, students should be comfortable with PilotScript and have the ability to use PilotScript to manipulate properties.

Topics	Details
<ul style="list-style-type: none">• Manipulating property values, lists, and names• Conditional statements and loops• Working with numbers and strings• Local and global variables• Anonymous property list functions• Debugging• String functions and regular expressions• Hash tables	<p>Duration: 0.5 Day</p> <p>Method: Onsite, Virtual Classroom, eLearning</p> <p>Level: Intermediate</p> <p>Prerequisites: Fundamentals</p>

PIPELINE PILOT INTEGRATION

This course provides students with the knowledge needed to utilize the scripting and 3rd-party integration functionality included in Pipeline Pilot. Topics covered include connecting to databases, RunProgram, SOAP and Web Services, API integration, and optionally VBScript, Perl or Java topics. Upon completion of the workshop, students will be able to modify and create complex components and protocols utilizing Pipeline Pilot's wide variety of integration capabilities.

Topics	Details
<ul style="list-style-type: none">• Server-Side Integration<ul style="list-style-type: none">– Databases and ODBC/JDBC– Command line components– SOAP and Web services– Language-based components (VBScript, Perl, Java)• Client-Side Integration<ul style="list-style-type: none">– Running protocols from the command line– Client SDKs (Java, .NET, JavaScript, SOAP)	<p>Duration: 0.5 Day Method: Onsite, Virtual Classroom, eLearning (Note: eLearning covers only server-side integration) Level: Advanced Prerequisites: Fundamentals, PilotScript</p>

BIOVIA FOUNDATION ADMINISTRATION

This course is perfect for individuals tasked with the administration of the Pipeline Pilot server and clients. Students learn how to install the server and clients, set up security, share and manage the XMLDB, and more. Upon completion of the workshop, students have the knowledge necessary to successfully set up and administer the Pipeline Pilot server and client.

Topics	Details
<ul style="list-style-type: none">• Installing and upgrading of BIOVIA Foundation• Running the Administration Portal• Apache Web Server• Setup and configuration• Security• Managing protocol jobs• Backing up, restoring and purging the XMLDB• Configuring databases	<p>Duration: 0.5 Day Method: Onsite, Virtual Classroom, eLearning Level: Intermediate Prerequisites: None</p>

CHEMISTRY

This course focuses on various components in the Pipeline Pilot Chemistry Collection. The components are reviewed by examining their parameters and how to use them. Exercises throughout the course demonstrate various uses of the collection such as physical property calculation, library enumeration, clustering, SAR analysis, and MCSS. These functionalities can be used to build protocols; triage screening results; generate, evaluate, and prioritize synthetic targets; and many other useful applications. Upon completion of the workshop, students will be able to modify and create complex protocols utilizing Pipeline Pilot's wide variety of scientific functionality.

Topics	Details
<ul style="list-style-type: none">• Calculating molecular properties• Manipulating molecules• Calculating molecular fingerprints• Substructure searching and similarity• Enumerating molecules (and create SAR table)• Cluster molecules• Maximal common substructure	<p>Duration: 1 Day Method: Onsite, Virtual Classroom, eLearning Level: Intermediate Prerequisites: Fundamentals, PilotScript</p>

DOCUMENTS AND TEXT

The Pipeline Pilot Documents and Text Collection unifies search, analysis, and reporting of diverse literature sources. This course covers the use of the collection. Upon completion of the workshop, students will have the knowledge necessary to modify and create protocols utilizing the Pipeline Pilot Text Analytics Collection.

Topics	Details
<ul style="list-style-type: none">• Searching remote databases, and local files and databases• Using concept dictionary/ontologies• Adding annotation• Using natural language processing• Applying analytics - correlation/trends• Document data modeling• Finding chemical names• Converting names to structures	<p>Duration: 1 Day Method: Onsite, Virtual Classroom Level: Advanced Prerequisites: Fundamentals, PilotScript</p>

DATA MODELING

This course covers both introductory and advanced topics associated with data modeling. This is NOT a statistics course. Students are led through the use of statistics to determine the relationships among their data for the purpose of understanding or prediction.

Topics	Details
<ul style="list-style-type: none">• Generic Statistics Components• Clustering• Regression Models• Bayesian Models• Recursive Partitioning• Pareto Optimization• Genetic Function Approximation	<p>Duration: 1 Day Method: Onsite, Virtual Classroom Level: Advanced Prerequisites: Fundamentals, PilotScript</p>

R STATISTICS COMPONENTS

This course covers the use of the R Statistics Collection for Pipeline Pilot. This is NOT a statistics course. However, students will learn the scope of the R component collection, how the components work, how to process the results, and how to build customized R components. The course is intended for Pipeline Pilot users already familiar with customizing components and developing custom protocols. Upon completion of the workshop, students will have the ability to modify and create complex protocols using the R Statistics component collection.

Topics	Details
<ul style="list-style-type: none">• Plotting• Analysis• Clustering• Learning• Custom R Script	<p>Duration: 0.5 Day Method: Onsite, Virtual Classroom Level: Advanced Prerequisites: Fundamentals, PilotScript</p>

SEQUENCE ANALYSIS

This course covers the use of the Pipeline Pilot Sequence Analysis Collection and is intended for users already familiar with customizing components and developing custom protocols. Upon completion of the workshop, students will have the ability to modify and create complex sequence analysis protocols utilizing Pipeline Pilot's wide variety of scientific functionality available in the Sequence Analysis Collection.

Topics	Details
<ul style="list-style-type: none">• Collection Basics• Annotations and Features• Search and Similarity<ul style="list-style-type: none">– Alignments– BLAST & HMMs– Entrez and DAS Utilities• Integration Tools<ul style="list-style-type: none">– 3rd Party Tools– BioJava• Perl & BioPerl	<p>Duration: 0.5 Day Method: Onsite, Virtual Classroom Level: Advanced Prerequisites: Fundamentals, PilotScript</p>

NEXT GENERATION SEQUENCING (NGS) PRIMER

This course provides a primer in Next Generation Sequencing (NGS) technologies for users who may have a biological background, but are not familiar with NGS. Students learn about current NGS methods in use, the types of data and data files produced by NGS experiments, and scientific questions that can be answered using NGS.

Topics	Details
<ul style="list-style-type: none">• Molecular Biology Review• NGS Overview• Sequencing Systems• Sequencing Data• Types of Sequencing• Applications	<p>Duration: 0.5 Day Method: Onsite, Virtual Classroom Level: Advanced Prerequisites: Fundamentals, PilotScript, basic understanding of biology</p>

BASIC NEXT GENERATION SEQUENCING (NGS)

This course introduces users to the Next Generation Sequencing (NGS) repository and some of the basic NGS components. The NGS repository serves as the central data and metadata storage hub for NGS experiments, reference sequences, features, variants, and other data types. In addition to learning how to create, manage, and work with their NGS repository, students will be introduced to the NGS collection's mapping, variant detection, and reporting components.

Topics	Details
<ul style="list-style-type: none">• Building a Repository• Analysis: SNP Detection• Viewers• Optional Topics<ul style="list-style-type: none">– Reporting Tools– Mapping Components– de novo Assembly– Variant Detection (including structural variation)• Useful Information<ul style="list-style-type: none">– Repository Scope– Paired End Reads for Illumina• Performance	<p>Duration: 0.5 Day Method: Onsite, Virtual Classroom Level: Advanced Prerequisites: Fundamentals, PilotScript, Sequence Analysis, basic understanding of NGS technology</p>

ADVANCED NEXT GENERATION SEQUENCING (NGS)

This course is a follow-on to the Basic Next Generation Sequencing (NGS) course and builds upon those lessons learned. Topics covered include advanced repository management, performing quality control on reads, extracting data and metadata from the repository, and using the components to analyze ChIP-Seq data. Advanced topics such as performance optimization and file management are also covered.

Topics	Details
<ul style="list-style-type: none">• Sequence Repository<ul style="list-style-type: none">– Create– Repository tools (rename, delete)– Queries• RNA-Seq<ul style="list-style-type: none">– Cufflinks– Cuffcompare– Cuffdiff• Useful information/Further work<ul style="list-style-type: none">– Chip-seq– Filters and manipulators– de novo Assembly– Performance	<p>Duration: 0.5 Day Method: Onsite, Virtual Classroom Level: Advanced Prerequisites: Fundamentals, PilotScript, Sequence Analysis, Basic NGS, understanding of NGS technology</p>

BASIC IMAGING

This course is designed for anyone wanting to use the Pipeline Pilot Imaging Collection. Students learn about data input, structure, manipulations, statistics, and reporting. Hands-on exercises assist students with gaining a firm grasp on the collection.

Topics	Details
<ul style="list-style-type: none">• Image Processing - Image and pixel manipulation<ul style="list-style-type: none">– Geometric: Rotate, translate, etc.– Change image appearance: Removing noise, smoothing, improving contrast, etc.• Image Analysis<ul style="list-style-type: none">– Finding objects in images– Performing measurements– Classifying objects or images	<p>Duration: 0.5 Day Method: Onsite, Virtual Classroom Level: Advanced Prerequisites: Fundamentals, PilotScript</p>

IMAGE ANALYSIS BASICS

This course is designed for non-imaging experts who would like to become familiar with image analysis using comprehensive examples and hands-on exercises. Students learn about sequences and stacks, intensity transformation, spatial filtering, segmentation, machine learning, and more.

Topics	Details
<ul style="list-style-type: none">• Image channels, sequences and stacks• Intensity transformation• Spatial filtering• Segmentation• Learning and clustering	<p>Duration: 0.5 Day Method: Onsite, Virtual Classroom Level: Advanced Prerequisites: Fundamentals, PilotScript, Basic Imaging</p>

ADVANCED IMAGING

This course is designed for imaging experts and takes a deep dive into the advanced features of the Imaging Collection: pixel manipulation, segmentation, object operations, colocalization, machine learning, 3D stacks, BigImage, and more. Hands-on exercises enhance the learning experience.

Topics	Details
<ul style="list-style-type: none">• Morphology components• Math and statistics components• Object manipulation components• Transforms• Learning and clustering components• Sequence and stack manipulation components	<p>Duration: 1 Day Method: Onsite, Virtual Classroom Level: Advanced Prerequisites: Fundamentals, PilotScript, Basic Imaging, Image Analysis Basics</p>

MOLECULAR TOOLKIT

The Molecular toolkit is a software development kit for accessing and modifying molecular data objects in protocols such as atoms, bonds, molecules, reactions and macromolecules. The toolkit is implemented in PilotScript, Perl and Java programming languages and is well suited for extending the native chemistry capabilities of Pipeline Pilot with custom methods.

Upon completion of the workshop, students will have the ability to create highly customized components that manipulate molecular objects in Pipeline Pilot.

Topics	Details
<ul style="list-style-type: none">• Create new molecules• Manipulate atoms• Manipulate bonds• Create new calculable properties	<p>Duration: 0.5 Day Method: Onsite, Virtual Classroom Level: Advanced Prerequisites: Fundamentals, PilotScript, Integration, Chemistry</p>

PLATE DATA ANALYTICS

The Pipeline Pilot Plate Data Analytics Collection extracts, analyzes, and reports on data from plate-based assays, including but not limited to single measurements, dose-response data, kinetic data, multiplex data, HCS images, and HTS molecules. Upon completion of the workshop students will have the ability to modify and create protocols utilizing the Pipeline Pilot Plate Data Analytics Collection.

Topics	Details
<ul style="list-style-type: none">• Create custom readers• Report and view plate data• Combine and split plates• Manipulate well properties• Create Dilution Series• Perform curve fitting• Calculate any ECx values• Identify hits or outliers• Normalize data• Calculate plate and well statistics	<p>Duration: 0.5 Day Method: Onsite, Virtual Classroom Level: Advanced Prerequisites: Fundamentals, PilotScript</p>

EXTENDING BIOVIA WORKBOOK WITH PIPELINE PILOT PROTOCOLS

Developed for Protocol developers with Pipeline Pilot experience or those who have completed the Building Pipeline Pilot Protocols class, this class teaches developers to record, organize and secure experimental information to find, share, and reuse critical knowledge globally. Using Pipeline Pilot can greatly increase the functionality of BIOVIA Workbook.

This workshop teaches students how to:

- Integrate Pipeline Pilot into BIOVIA Workbook.
- Allow template builders to extend the functionality of the BIOVIA Workbook with protocols built using all the collections available in Pipeline Pilot.
- Easily connect BIOVIA Workbook menus and buttons to Pipeline Pilot protocols.

Topics	Details
<ul style="list-style-type: none">• Build an BIOVIA Workbook template• Build protocols<ul style="list-style-type: none">– BIOVIA Workbook components– Data exchange conventions– Retrieve data using buttons in experiments– Analyze tab• Configure protocols to run from an experiment• Publish and maintain protocols	<p>Duration: 0.5 Day Method: Onsite, Virtual Classroom Level: Advanced Prerequisites: Fundamentals, PilotScript, BIOVIA Workbook</p>

ELEARNING LIBRARY

Pipeline Pilot offers a full suite of eLearning courses. You can purchase the entire suite on a per-user basis, for a one-year duration. Contact your Account Manager for details.

Information on the content provided in each course is provided here.

FUNDAMENTALS OF PIPELINE PILOT

Introduction to Pipeline Pilot

Explanation of how Pipeline Pilot can assist the user in automating everyday tasks. Those new to the software can gain an understanding of its uses through this module.

Creating Your First Pipeline

Get started with Pipeline Pilot. You will learn how to build your own protocols, and configure parameters on components so they work with the data you choose.

Tour of the Pro Client

Become acquainted with the layout of the Pipeline Pilot Pro Client. The Pro Client is used by developers to run and develop protocols.

Design Mode, Checkpoints, and Debugging a Pipeline

Learn about the debugging capabilities within Pipeline Pilot. These include Pipeline Pilot's checkpoint capabilities, Design Mode, Debug Mode, and the Protocol Comparison functions.

Anatomy of a Component Collection

Identify the basic parts of a component, review working with components in a pipeline, and identify the basic types of components and their functions.

Filters - Control of Flow

Learn about components to filter data. Filters are used to divide the records on the data stream based on specified criteria. Records that match the criteria are sent out the pass port while those that do not are sent out the fail port. Filters can be used to remove records from the data stream, separate records into two streams, or to test that a property is present on the data record.

Merging Data in a Pipeline

Learn about the components that merge data. Merging data combines records on the data stream based on specified criteria, a key. The key is one or more properties from the data stream.

Joining Data in a Pipeline

Joining data is a way to add properties to records on the data stream. Properties are added to data records from a reference cache or a file based on a key, one or more properties.

Grouping Data

Grouping data in Pipeline Pilot is a way to reversibly aggregate data together either by number of records or by a key property.

Differences between Merging, Joining, and Grouping

Explanation of the different types of output you will receive when you utilize the merge, join, and group components.

Introduction to PilotScript

Learn about PilotScript, the native scripting language in Pipeline Pilot. PilotScript is used in Custom Filters and Custom Manipulators to allow more powerful data manipulation.

Subprotocols

Instructions using a subprotocol to collapse one or more components into a single item. You will learn how to create a subprotocol, how to add or expose parameters on it, and share it as a reusable component.

Run to Completion Subprotocols

Explanation of the difference between the data flow in a subprotocol and a Run to Completion subprotocol. You also learn how this can add function to your protocols.

Passing Data between Pipelines

Sometimes it is essential to have more than one pipeline in a protocol. Here you will discover how data passes between multiple pipelines. We recommend that you take the *Filters - Control of Flow*, *Merging Data*, *Joining Data*, *PilotScript*, and *Run to Completion Subprotocols* modules as prerequisites.

Web Port

Review of Pipeline Pilot Web Port, a web-based application for running protocols in a browser. This allows users to run protocols from remote locations where they cannot access a Pipeline Pilot client. You will learn basic Web Port publishing in this module. For information on how to use the reporting collection to create form and work protocols that can be published to Web Port, refer to the *Pipeline Pilot Reporting* eLearning module.

Running Pipelines Automatically

Learn how to run Pipeline Pilot protocols automatically. Pipeline Pilot has the capacity to run through a command line prompt. This can be utilized to allow scheduling of protocol execution through the Windows Task Scheduler, or via a cron job in Linux.

Additional Topics

Covers technical support, client-server architecture, and temporary files.

PIPELINE PILOT ADMINISTRATION PORTAL

Essential Portal Functions

This module shows you how to utilize the essential functions of the Pipeline Pilot Administration Portal, which is a collection of online tools for system administrators who need to manage servers and clients. The portal is a web application that provides secure access from any network location, independent of the server. Those taking this course should be administrators or have permission to alter administrative settings.

PIPELINE PILOT PILOTSRIPT

Introduction

Throughout this course, you will utilize the two main PilotScript components -- there are others in Pipeline Pilot that work in a similar manner. In this module, you are introduced to PilotScript, the native scripting language of Pipeline Pilot. You will learn how PilotScript can help you improve protocols, and the basics of using a scripting language.

Filtering and Manipulating Data Records

Learn property naming conventions and management functions, how to filter data sets, and how to manipulate property values.

Data Record Properties

Learn the characteristics of data record properties, how to reference them in PilotScript -- including the deep properties that are used with imaging and text analytics -- and how to access a data record's property list without identifying specific property names.

Statement Building Blocks

Learn how to use the building blocks of statements -- arithmetic operators and strings, conditionals and loops, and date and time functions.

Variables, Arrays, and Hash Tables

Learn what variables and arrays are, and the basics of using them in statements. You will also learn how to create and utilize hash tables.

Debugging

Learn protocol debugging tips, functions, modes, and components.

PIPELINE PILOT INTEGRATION

Server-Side Integration

This course shows you how to use key components in the Integration collection. These components allow you to extend the functionality of Pipeline Pilot Server (PPS) by integrating third-party data and computational services on PPS. Those taking this course should have an understanding of databases, scripting languages, web services, and advanced protocol building skills.

PIPELINE PILOT REPORTING

Introduction

The Pipeline Pilot Reporting course covers the reporting components available in the Reporting and Visualization folder on the Components tab of Pipeline Pilot. There are also reporting components available that are specific to other component collections. The concepts in this course apply to those components as well. This module introduces you to using the reporting components.

Report Design and Layout

Covers the Paragraph, Bulleted List, Tiling, Page, Header, and Footer components, as well as using HTML tags with the Text component, style sheets, and combining static text and property values.

Tables

Introduces students to the variety of ways there are to build and present tables in reports.

Charts

Covers the chart components available in the Reporting and Visualization/Basic Reporting/Charts folder on the Components tab of Pipeline Pilot. Chart components are also available that are specific to other component collections. The concepts in this module also apply to those components.

Molecular Input Elements

Review of the two components you can use to edit and present live chemistry in your reports. The Chemistry Sketcher component allows you to sketch a molecule using your chemistry sketcher, and transfer it back into Pipeline Pilot as a chemistry object. The Discovery Studio Visualizer component adds a 3D display of a molecular object into an HTML report. To execute the tasks in this module, you need to have the Chemistry component collection installed on your Pipeline Pilot server.

Interactive Forms

Interactive forms allow you to create reports based on user input. In this module, you will learn how to use form components such as Text Box, List Box, Checkbox, Radio Button List, and File Chooser.

Dynamic Interactivity

Learn how to tell components, through scripting, to trigger interactive events in the output of your reporting protocols. Note that to execute the tasks in this module, you need to understand PilotScript and JavaScript.

Additional Interactive Reporting Tips and Tricks

Add links and simple dynamic interaction to reports, and publishing forms to Web Port.

Canvas Elements

Learn how to draw and label objects, in a defined working space, that work with your data -- giving you many options for enhancing your reports. Students should already have a working knowledge of how to use the Reporting collection to create reports and charts, and of PilotScript.

Working with Microsoft Office Products

Learn to use the Office Elements components to output a report to Word, Excel, and PowerPoint.

CHEMINFORMATICS

Introduction to Cheminformatics

Introduction to Pipeline Pilot's Chemistry collection of components and their general uses.

Calculation of Molecular Properties

Introduction to property calculators, calculable properties, and molecular fingerprints.

Manipulating Molecules

Description of chemistry data manipulator components that alter data records in a variety of ways, including cleaning, structural altering, and standardizing.

Molecular Filters

Discussion of filters that act on molecular data, allowing customization of your workflows to incorporate processing according to the chemical and structural features of a molecule on a data record.

Substructure Searching and Molecular Similarity

Instruction on how you can use various components to perform database-style searching of molecules, and to identify similarities among them. The use and purpose of these tasks will also be discussed. Note that to execute the tasks in this module, you need to have the Data Modeling component collection installed on your Pipeline Pilot server.

Estimation and Visualization

Learn to use components that analyze research data and present the results in a meaningful manner. Specifically, you will use components that create relationship tables, cluster data sets, and estimate pKa and logD values for molecules. Note that to execute the tasks in this module, you need to have the Data Modeling Component Collection installed on your Pipeline Pilot server.

Enumerating Tautomers and Stereochemistry

Review of what tautomers and stereochemistry are, and how to use Pipeline Pilot components with these types of structures.

Reactions

Discussion of performing reactions with a protocol on individual molecules, on a set of starting materials, and using a core structure. Enumeration methods for each of these types of reactions are also covered

Bioisosteres

This module will review what bioisosteres are, how they are used in chemistry research, and the main components Pipeline Pilot offers for discovering and working with bioisosteres.