

BIOVIA Pipeline Pilot

Training Course Catalog



3DEXPERIENCE®

PIPELINE PILOT COURSE CATALOG

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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:** Facilitated by an instructor, this training takes place at your location or through a virtual classroom. Onsite courses offer hands-on exercises to enhance the learning experience. In remote classes, hands-on exercises are assigned as homework, rather than during class time.
- **eLearning:** These self-paced, computer-based courses cover most BIOVIA Pipeline Pilot-specific topics that you can use as a supplement to the instructor-led training or as a primary source for learning. A description of each module available in the package is included in this catalog. Note that eLearning is sold separately.

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>Onsite Training: 1 Day</p> <p>Remote Training: Two 3-Hour Sessions</p> <p>eLearning: Available (see page 10)</p> <p>Level: Beginner</p> <p>Prerequisites: None</p>

BIOVIA FOUNDATION ADMINISTRATION

The capabilities of BIOVIA Foundation Hub to centrally manage BIOVIA applications across the enterprise are introduced in this course. Administrators will learn how to manage users, groups, and permissions and integrate with existing Active Directory or LDAP servers. Storing information such as equipment, locations, projects, and units will also be covered. Subsequent sections detail the automated management using protocols, components and APIs.

Topics	Details
<ul style="list-style-type: none">• Security<ul style="list-style-type: none">– Creating and importing users– Groups and permissions– External claims and LDAP• Equipment, units and vocabularies• Pipeline Pilot protocols and components• BIOVIA Foundation Hub APIs• Installation of BIOVIA Foundation Hub	<p>Onsite Training: 1 Day</p> <p>Remote Training: Two 3-Hour Sessions</p> <p>eLearning: Available (see page 12)</p> <p>Level: Intermediate</p> <p>Prerequisites: None</p>

PIPELINE PILOT 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">• Deployment• Apache Web Server• Setup and configuration• Security• Clusters and grids• Load balanced deployment• Managing protocol jobs• Backing up, restoring, and purging the XMLDB• Catalog & Server Registry• Configuring databases	<p>Onsite Training: 0.5 Day</p> <p>Remote Training: 3 Hours</p> <p>eLearning: Not Available</p> <p>Level: Intermediate</p> <p>Prerequisites: None</p>

REPORTING AND INTERACTIVE REPORTING

This course covers the use of the Pipeline Pilot Reporting Collection. Topics cover using static and 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<ul style="list-style-type: none">– Tables– Charts– Conditional formatting– Interactivity – tooltips, hyperlinks, etc.• Creating input forms to run protocols from a browser	<p>Onsite Training: 1 Day</p> <p>Remote Training: Two 3-Hour Sessions</p> <p>eLearning: Available (see page 13)</p> <p>Level: Intermediate</p> <p>Prerequisites: Pipeline Pilot 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>Onsite Training: 0.5 Day</p> <p>Remote Training: 3 Hours</p> <p>eLearning: Available (see page 15)</p> <p>Level: Intermediate</p> <p>Prerequisites: Pipeline Pilot Fundamentals</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>Onsite Training: 1 Day</p> <p>Remote Training: Two 3-Hour Sessions</p> <p>eLearning: Available (see page 16)</p> <p>Level: Intermediate</p> <p>Prerequisites: Pipeline Pilot Fundamentals, PilotScript</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>Onsite Training: 0.5 Day</p> <p>Remote Training: 3 Hours</p> <p>eLearning: Available for server-side integration only (see page 14)</p> <p>Level: Advanced</p> <p>Prerequisites: Pipeline Pilot 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>Onsite Training: 1 Day</p> <p>Remote Training: Not Available</p> <p>eLearning: Not Available</p> <p>Level: Advanced</p> <p>Prerequisites: Pipeline Pilot Fundamentals, PilotScript</p>

PIPELINE PILOT ANALYTICS AND MACHINE LEARNING

This course covers both introductory and advanced topics associated with Pipeline Pilot analytics and machine 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>Onsite Training: 1 Day</p> <p>Remote Training: Not Available</p> <p>eLearning: Not Available</p> <p>Level: Advanced</p> <p>Prerequisites: Pipeline Pilot 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>Onsite Training: 0.5 Day</p> <p>Remote Training: 3 Hours</p> <p>eLearning: Not Available</p> <p>Level: Advanced</p> <p>Prerequisites: Pipeline Pilot 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>Onsite Training: 0.5 Day</p> <p>Remote Training: 3 Hours</p> <p>eLearning: Not Available</p> <p>Level: Advanced</p> <p>Prerequisites: Pipeline Pilot Fundamentals, PilotScript</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– <i>de novo</i> Assembly– Variant Detection (including structural variation)• Useful Information<ul style="list-style-type: none">– Repository Scope– Paired End Reads for Illumina• Performance	<p>Onsite Training: 0.5 Day</p> <p>Remote Training: 3 Hours</p> <p>eLearning: Not Available</p> <p>Level: Advanced</p> <p>Prerequisites: Pipeline Pilot 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">– 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– <i>de novo</i> Assembly– Performance	<p>Onsite Training: 0.5 Day</p> <p>Remote Training: 3 Hours</p> <p>eLearning: Not Available</p> <p>Level: Advanced</p> <p>Prerequisites: Pipeline Pilot 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>Onsite Training: 0.5 Day</p> <p>Remote Training: 3 Hours</p> <p>eLearning: Not Available</p> <p>Level: Advanced</p> <p>Prerequisites: Pipeline Pilot Fundamentals, PilotScript</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>Onsite Training: 1 Day</p> <p>Remote Training: Two 3-Hours Sessions</p> <p>eLearning: Not Available</p> <p>Level: Advanced</p> <p>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>Onsite Training: 0.5 Day</p> <p>Remote Training: 3 Hours</p> <p>eLearning: Not Available</p> <p>Level: Advanced</p> <p>Prerequisites: Fundamentals, PilotScript, Integration, Chemistry</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>Onsite Training: 0.5 Day</p> <p>Remote Training: Not Available</p> <p>eLearning: Not Available</p> <p>Level: Advanced</p> <p>Prerequisites: Pipeline Pilot 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 pricing and additional information.

PIPELINE PILOT FUNDAMENTALS

This curriculum familiarizes students with building and utilizing protocols in Pipeline Pilot. Protocols are pipelines of process steps you use to rapidly create, test, and publish scientific services and automate the process of accessing, analyzing, and reporting scientific data. All modules contain exercises and quizzes.

Fundamentals Introduction

In Fundamentals you will learn the many uses of Pipeline Pilot, and how it helps automate everyday tasks. You'll learn the interface layout, how to build protocols, and how to configure parameters on components so they work with the chosen data.

Topics covered:

- Exploring Pipeline Pilot
- Exploring the Layout
- Building a Protocol
- Reviewing the Client-Server Architecture

Manipulate Components

Discover the basics of components and how you can work with them in a pipeline.

Topics covered:

- Exploring Components and Parameters
- Adding Components to a Pipeline
- Working with Existing Components

Debug a Pipeline

Learn how you can use Pipeline Pilot's debugging capabilities.

Topics covered:

- Utilizing Checkpoints
- Viewing Design Mode
- Utilizing Debugging Tools
- Managing Protocol Versions
- Comparing Protocols

Filter Data

Explore how you can use filters to remove records from your data stream, separate records into two streams, and test that a property is present on your data record.

Topics covered:

- Browsing Filters
- Filtering by the Value of a Property
- Defining a Property

Merge Data

Learn to combine records based on one or more specified properties from the data stream, known as a key. You will also learn the different types of output you receive when you use the merge, join, and group components.

Topics covered:

- Browsing the Merge Components
- Combining Data Records with a Key
- Merging Properties of all Input Data Records
- Comparing Merging, Joining, and Grouping

Join Data

Discover how to add properties to your data records from a reference cache or a file based on one or more specified properties from the data stream, known as a key. You will also learn the different types of output you will receive when you utilize the merge, join, and group components.

Topics covered:

- Adding Properties to Records on the Data Stream
- Comparing Merging, Joining, and Grouping

Group Data

Learn how to reversibly aggregate data together either by number of records or by a key property. You will also learn the different types of output you will receive when you utilize the merge, join, and group components.

Topics covered

- Grouping Data by a Tag
- Filtering Grouped Data
- Grouping Data by a Set Number of Records
- Comparing Merging, Joining, and Grouping

Utilize PilotScript

PilotScript is the native scripting language in Pipeline Pilot that allows for the powerful manipulation of data records and control of data flow within pipelines. This course provides Instruction on how to use PilotScript, as well as how to add PilotScript to custom filters and custom manipulators.

Topics covered

- Using the PilotScript Editor
- Filtering Data Sets
- Accessing Calculable Properties and Functions
- Reviewing Comparisons, Variable Types, and Property Lists

Create Subprotocols

Learn to create a subprotocol to collapse one or more components into a single item. You're also taught to add or expose parameters on a subprotocol, and share it as a reusable component. Discover the difference between the data flow in a subprotocol and a Run to Completion subprotocol, and how this can add functionality to your protocols.

Topics covered:

- Combining Components into a Subprotocol
- Editing a Subprotocol
- Saving and Sharing a Subprotocol
- Running to Completion

Pass Data between Pipelines

Explore the use of global variables, caches, files, and temporary files to pass data between multiple pipelines.

Topics covered:

- Running Multiple Pipelines
- Passing Data with Global Variables, with Caches, and with Files
- Reviewing File Locations

Run and Automate Protocols Outside of Pipeline Pilot

Discover Pipeline Pilot Web Port, a web-based application for running protocols in a browser. You are also taught to run protocols automatically through a command line prompt, and then schedule protocol execution through the Windows Task Scheduler, or via a cron job in Linux.

Topics covered:

- Working with Web Port
- Running a Protocol from a Windows Command Line
- Scheduling a Protocol Job

PIPELINE PILOT ADMINISTRATION

Instruction on using the Pipeline Pilot Administration Portal, a collection of online tools for system administrators who need to manage servers and clients. Those taking this course should be administrators or have permission to alter administrative settings. All modules contain exercises and quizzes.

Topics covered:

- Exploring the Administration Portal
- Managing Security Settings
- Setting up and Searching the XMLDB Catalog
- Defining and Administering Databases

PIPELINE PILOT REPORTING

This curriculum focuses on the reporting components available in the Reporting and Visualization folder on the Components tab of Pipeline Pilot. You can apply the concepts presented in this curriculum to other Pipeline Pilot reporting collections. All modules contain exercises and quizzes.

Reporting Introduction

Introduction to the Pipeline Pilot reporting components.

Topics covered:

- Exploring the Reporting Collection
- Reviewing Reporting Data Structure and Basic Reporting Components

Manipulate the Design and Layout of Reports

Instruction on using the paragraph, bulleted list, tiling, page, header, and footer components. You also learn about stylesheets, combining static text and property values, and using HTML tags with the Text component.

Topics covered:

- Creating Paragraphs, Bulleted Lists, Stylesheets
- Tiling Report Elements
- Laying out Pages
- Creating Headers and Footers
- Manipulating Property Values
- Allowing HTML Tags on the Text Component

Utilize Tables

Instruction on a variety of ways available to build and present tables in reports.

Topics covered:

- Reviewing Table Basics
- Building Interactive Tables
- Building Paged Tables

Create Charts

Learn to use the chart components available in the Reporting and Visualization\Basic Reporting\Charts folder on the Components tab of Pipeline Pilot. Concepts derived from this course can be applied to chart components that are specific to other component collections.

Topics covered:

- Adding and Customizing Charts
- Reviewing Charting Components

Insert Molecular Input Elements

Learn how to use the two components that present live chemistry in reports. Note that to execute the tasks in this module, you must have the Chemistry component collection installed on your Pipeline Pilot server.

Topics covered:

- Sketching Molecules
- Displaying 3D Molecules

Build Interactive Forms

Learn to create reports that are based on user input, and how to publish forms to Web Port.

Topics covered:

- Reviewing Form and Work Protocols
- Building a Form and Working with Form Components
- Publishing Interactive Forms to Web Port

Add Dynamic Interactivity to Forms

Instruction on how to add simple and complex dynamic interaction to reports. Note that to execute some of the tasks in this course, you must already have an understanding PilotScript and JavaScript.

Topics covered:

- Utilizing Simple Interactivity
- Utilizing Complex Activity

Utilize Canvas Elements

Learn how to draw and label objects in a defined working space, that work with specific data -- providing many options for enhancing reports. Before starting this course, students should already have a working knowledge of PilotScript, as well as how to use the Pipeline Pilot Reporting collection to create reports and charts.

Topics covered:

- Creating a Canvas
- Adding Content to an XY Chart

Work with Microsoft Office Products

This course teaches you how to use the Office Elements components to output a report to Word, Excel, and PowerPoint.

Topics covered:

- Outputting Data to Word and Excel
- Outputting Data to Powerpoint

PIPELINE PILOT INTEGRATION

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

Topics covered:

- Reading Data Stored in an External Database into a Protocol
- Running Program Command Lines on the Server
- Executing Basic Language Commands on the Server
- Reading Data from Web Services into a Protocol

PIPELINE PILOT PILOTSRIPT

This curriculum focuses on PilotScript -- Pipeline Pilot's functional expression language used to design custom components. You will design components that filter and manipulate data, access data record properties and variables, and debug protocols. Throughout this curriculum, you will utilize the two main PilotScript components -- there are others in Pipeline Pilot that work in a similar manner. All modules contain exercises and quizzes.

Pipeline Pilot Introduction

Introduction to PilotScript, the native scripting language of Pipeline Pilot. You'll learn the basic of using a scripting language, and how PilotScript can help improve protocols.

Topics covered:

- Exploring PilotScript
- Reviewing Scripting Basics
- Utilizing the Expression Editor

Filter and Manipulate Data Records

Provides definitions of the property naming conventions and management functions, as well as instruction on how to filter data sets, and how to manipulate property values.

Topics covered:

- Filtering Data Sets
- Manipulating Property Values

Work with Data Record Properties

Instruction on 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.

Topics covered:

- Utilizing Properties in PilotScript
- Working with Anonymous Property List Functions
- Reviewing Deep Properties

Utilize Statement Building Blocks

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

Topics covered

- Utilizing Arithmetic Operators and Strings
- Adding Conditionals and Loops to Statements
- Reviewing Date and Time Functions

Work with Variables, Arrays, and Hash Tables

Definitions of variables and arrays, and instruction on the basics of using them in PilotScript statements. You'll also learn how to create and utilize hash tables.

Topics covered:

- Exploring Global and Local Variables
- Accessing Data Review Values in an Array
- Adding Hash Functions to Statements

Debug Protocols

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

Topics covered:

- Debugging Functions and Running Protocols in Debug Mode
- Working in Design Mode
- Reviewing Debugging Components

PIPELINE PILOT CHEMINFORMATICS

This curriculum focuses on Pipeline Pilot's Chemistry collection and how to utilize these tools to deploy Pipeline Pilot in a chemistry setting. Students will learn to use components to perform compound processing and cheminformatics research and analysis. All modules contain exercises and quizzes.

Cheminformatics Introduction

An introduction to Pipeline Pilot's Chemistry collection of components and their general uses. You'll also be instructed on chemistry data manipulator components that alter data records in a variety of ways, including cleaning, structural altering, and standardizing.

Topics covered:

- Exploring the Chemistry Collection
- Reviewing Common Chemistry Manipulators

Calculate Molecular Properties

Learn to use property calculators, calculable properties, and molecular fingerprints.

Topics covered:

- Working with Property Calculators
- Utilizing the Molecular Fingerprints Component

Filter Molecules

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

Topics covered:

- Reviewing the Filters
- Modeling Data
- Accessing and Manipulating Data
- Similarity

Perform Molecule Searches and Identify Similarities

Learn to utilize various components to perform database-style searching of molecules, and to identify similarities among them. Note that to execute the tasks in this course, you must have the Data Modeling component collection installed on your Pipeline Pilot server.

Topics covered:

- Reviewing the Search and Similarity Components
- Checking Molecules for Query Substructures
- Finding Molecules Similar to the Query Structure
- Constructing a Query
- Generating Maximal Common Substructure
- Calculating Similarity Values

Estimate and Visualize

Learn how to use components that analyze research data and present the results in a meaningful manner. Note that to execute the tasks in this module, you must have the Data Modeling component collection installed on your Pipeline Pilot server.

Topics covered:

- Generating SAR Information
- Clustering
- Estimating logD and pKa

Enumerate Tautomers and Stereochemistry

Provides descriptions of tautomers and stereochemistry are, and instructs you on how to use Pipeline Pilot components with these types of structures.

Topics covered

- Enumerating Tautomers
- Enumerating Stereoisomers

Perform Reactions

Instruction on how to use reactions with a protocol on individual molecules, on a set of starting materials, and on using a core structure. You'll also receive instruction on the enumeration methods for each of these types of reactions.

Topics covered:

- Reviewing Reaction Components
- Working with Reaction-Based Enumeration
- Working with Scaffold-Based Enumeration

Explore and Work with Bioisosteres

Provides descriptions of bioisosteres, how they are used in chemistry research, and the main components Pipeline Pilot offers for discovering and working with bioisosteres.

Topics covered

- Reviewing Bioisosteres Components
- Identifying and Enumerating Bioisosteres
- Reviewing Similarity Bioisosteres
- Utilizing the Similarity Components