BIOVIA Discovery Studio

2017 Training Course Catalog

3DEXPERIENCE®

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SUMMARY

We are proud to offer a variety of courses to meet your organization's needs. Customized courses can be designed to meet your team's specific needs; please contact your Account Manager for more information.

Course Delivery Methods

- **Onsite Instructor-Led Training**: Facilitated by an onsite instructor, this training takes place at your location or at a selected Biovia site. Onsite courses offer hands-on exercises to enhance the learning experience.
- **WebEx Instructor-Led Training**: Our instructors teach these courses remotely, using WebEx, allowing students to attend from their own location by logging in to the WebEx site. In these classes, hands-on exercises are assigned as homework, rather than during class time.

INTRODUCTORY COURSES

INTRODUCTION TO DISCOVERY STUDIO

This course serves as a comprehensive introduction to the Biovia Discovery Studio software suite. The graphical interface and the various modules and modeling tools available within the software are described. Students become familiar with the software's configuration, running protocols, toolbars, command menus, and preferences. Different molecular displays and visualization modes including the data view, hierarchy view, sequence view, and data management storage and retrieval are discussed. The creation of story boards (movies), Active X, exporting graphics files, and 3D Web GL objects are demonstrated. Hands on exercises are included.

Topics	Course Duration and Prerequisites
• Modeling Applications Available Within Discovery Studio • Discovery Studio Architecture and Configurations • User Interface • Explorers (Tools, Protocol, Files) • Windows: Molecule, Sequence, Sequence Annotation, and Chart • Selection and Grouping • Working with Proteins • Running Protocols • Collaboration: Storyboards, ActiveX, exporting graphics files (*.json and *.dae), and sharing 3D objects on WebGL-enabled browsers • Customization: Scripting, Toolbars, Tool Sets, Tools Explorer, Tool Panel	**Onsite Training**: 1 Day **WebEx Training**: 3 Hours **Prerequisites:** • None

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DISCOVERY STUDIO PIPELINE PILOT INTEGRATION

This course provides a very basic overview of working with Pipeline Pilot components and introduces examples for different levels of DS protocol customization.

Topics	Course Duration and Prerequisites
• Customize (i.e., promote or de-promote) parameters of existing Discovery Studio protocols/components • Add or remove available components from existing Discovery Studio protocols/components • Create a new component and add to an existing Discovery Studio protocol • Increase automation of Discovery Studio protocols (e.g., automate protocol to run over all files in a specific folder) • Easily connect to an external relational database • Integrate third-party algorithms (e.g., CORINA, proprietary codes for descriptor calculations)	**Onsite Training:** 1 Day **WebEx Training:** 3 Hours **Prerequisites:** Introduction to Discovery Studio

SCRIPTING

Discovery Studio provides a client interface for working with a variety of documents and protocols. Occasionally, it may be desirable to access specific Discovery Studio functionality programmatically. Perl scripts enable you to perform certain tasks, by allowing you to manipulate objects in the application's environment, both at the command line and interactively.

Topics	Course Duration and Prerequisites
• Automate repetitive tasks • Link several tasks or calculations together in sequence • Explore calculations that are not available from any of the application's modules • Integrate with other software • Discussion of Perl scripting language	**Onsite Training:** 1 Day **WebEx Training:** Not available **Prerequisites:** Introduction to Discovery Studio

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PROTEIN-BASED MODELING

PROTEIN-PROTEIN DOCKING

This course covers the use of the ZDOCK protein-protein docking software and RDOCK energy rescoring programs available within the Discovery Studio suite. The ZDOCK methodology, as well as algorithms for clustering results are described. Methods for the use of guiding protein-protein docking available within Discovery Studio by filtering residues known experimentally to be involved at the protein-protein interface, as well as excluding those known not to be through blocking, are demonstrated.

Topics	Course Duration and Prerequisites
• The significance, importance, and challenges of performing computational protein-protein docking • ZDOCK and analysis • Refining the poses of RDOCK	**Onsite Training:** 1 Day **WebEx Training:** 3 Hours **Prerequisites:** Introduction to Discovery Studio

PROTEIN HOMOLOGY MODELING

This course introduces students to the theory of protein homology modeling and the tools available within Discovery Studio. Methods for selecting a protein template structure, aligning the template protein sequence to the target sequence, building the homology model, and assessing the quality of the protein structural model within the Discovery Studio framework are described. Methods available for refining the protein model within Discovery Studio are presented.

Topics	Course Duration and Prerequisites
• Assessing the limitations and assumptions in protein homology modeling • Selecting an appropriate protein structural template to create a model • Aligning your protein target sequence to a protein template sequence • Building a protein homology model using Discovery Studio 2016 tools • Analyzing the model in terms of quality, energy and structural features • Refining the homology model • Using the homology model for further studies, including mutagenesis studies, protein-protein docking, or ligand docking for structure-based drug design	**Onsite Training:** 1 Day **WebEx Training:** 3 Hours **Prerequisites:** Introduction to Discovery Studio

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ANTIBODY MODELING

This course instructs students in the application of the new Antibody Modeling Cascade available within Discovery Studio 2016. This method provides for automatic generation of a 3D model structure for antibody Fab or Fv regions starting from a set of five antibody structures. This course also provides instruction in the manual modeling and alignment tools for antibody structure, identifying framework templates and antibody loops, and the use of the Antibody Modeling Cascade. The use of Proteins 3D to verify the modeled antibody structures are also presented. Exercises for students to follow in modeling antibody examples are provided.

Topics	Course Duration and Prerequisites

• Introduction to antibodies
• Fab antibody modeling
  – Antibody Modeling Cascade
  – Identify Framework Templates
  – Model Antibody Framework
  – Model Antibody Loops
  – Graft Fab Structure
  – Model Bispecific Antibodies
• Full length antibody modeling
• Minimization
	Onsite Training: 1 Day
	WebEx Training: 3 Hours
	Prerequisites: Introduction to Discovery Studio

SIMULATIONS

This course focuses on working through the CHARMm, DelPhi, and CDOCKER Discovery Studio interfaces.

Topics	Course Duration and Prerequisites
• Energy calculations • Manual and automatic atom potential typing • Energy minimization • Molecular dynamics • Constraints • Solvation models • Trajectory analysis • Force field-based docking • Electrostatic calculations	**Onsite Training:** 1 Day **WebEx Training:** 4 Hours **Prerequisites:** Introduction to Discovery Studio

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QM/MM

The QM/MM course provides an overview of quantum mechanics, molecular mechanics and their combination in QM/MM calculations within Discovery Studio.

Topics	Course Duration and Prerequisites
• When to use QM/MM methods • Overview of density functional theory and its implementation in DMol^3 • Overview of molecular mechanics calculations with CHARMm • Considerations for the preparation and setup of QM/MM systems • Performing QM/MM calculations in Discovery Studio	**Onsite Training:** 1 Day **WebEx Training:** 3 Hours **Prerequisites:** Introduction to Discovery Studio

LIGAND-BASED DESIGN

PHARMACOPHORE MODELING IN DISCOVERY STUDIO

This course provides an introduction to pharmacophore modeling in Discovery Studio. It provides an overview of the diverse applications of these tools in drug discovery and design, and is the foundation for subsequent pharmacophore courses.

Topics	Course Duration and Prerequisites

• Pharmacophore definition and features
• Pharmacophore application in drug discovery
• Ligand-pharmacophore scoring and mapping
• Ligand perception
  – Conformation generation
  – Multi-conformer databases
	Onsite Training: 1 Day
	WebEx Training: 3 Hours
	Prerequisites: Introduction to Discovery Studio

3D QSAR PHARMACOPHORE GENERATION

This course covers the generation of quantitative pharmacophores in Discovery Studio, detailing the automated algorithms (HypoGen/HypoGenRefine) and the applications of these models in drug discovery and design

Topics	Course Duration and Prerequisites
• Creating 3D QSAR pharmacophores from activity data training sets • Refining pharmacophores with excluded volumes using data from inactive ligands • Analysis and application of quantitative pharmacophore	**Onsite Training:** 0.5 Day **WebEx Training:** 2 Hours **Prerequisites**: Introduction to Discovery Studio, Pharmacophore Modeling in Discovery Studio

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COMMON FEATURE PHARMACOPHORE GENERATION

This course covers the generation of qualitative pharmacophores in Discovery Studio, detailing the automated algorithms (HipHop/HipHopRefine) and the applications of these models in drug discovery and design.

Topics	Course Duration and Prerequisites
• Creating common feature pharmacophores from active ligand training sets • Generating pharmacophore-derived alignments of ligands • Using data from inactive ligands to add excluded volumes to pharmacophores to reduce false positives • Analysis and application of qualitative pharmacophores	**Onsite Training:** 0.5 Day **WebEx Training:** 2 Hours **Prerequisites:** Introduction to Discovery Studio • Pharmacophore Modeling in Discovery Studio

RECEPTOR-BASED PHARMACOPHORES

This course provides an overview of the approaches to deriving pharmacophores from receptor structures and presents their applications in diverse molecular modeling workflows. Students are guided through the steps required to create receptor-based pharmacophore models in Discovery Studio.

Topics	Course Duration and Prerequisites
• Automated protein-ligand pharmacophore generation • Multiple ligands alignment-based pharmacophores • Fragment-based pharmacophores for lead optimization • Structure-based pharmacophores from interactions maps • Validation and analysis of receptor-based pharmacophores	**Onsite Training:** 0.5 Day **WebEx Training:** 2 Hours **Prerequisites**: Introduction to Discovery Studio, Pharmacophore Modeling in Discovery Studio

FRAGMENT-BASED DRUG DESIGN IN DISCOVERY STUDIO

This course covers approaches for successful fragment-based lead optimization. Topics include fragment generation, analysis, and identification of fragment scaffolds from ligand libraries; as well as growing, replacing, and placing fragments within a protein target.

Topics	Course Duration and Prerequisites

• Introduction to Fragment-Based Drug Design
• Working with fragments and proteins in Discovery Studio
  – Preparation (**Re**trosynthetic **C**ombinatorial **A**nalysis **P**rocedure (ReCAP) approach)
  – Analysis
• Fragment-based drug design modes
  – REPLACE, GROW, PLACE
	Onsite Training: 1 Day
	WebEx Training: 3 Hours
	Prerequisites: Introduction to Discovery Studio

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LIBRARY DESIGN AND ANALYSIS

Ideally, compound libraries used for virtual high-throughput screening maximize diversity while optimizing key molecular properties. This course discusses the tools within Discovery Studio used to design, analyze, select subsets, and compare combinatorial libraries.

Topics	Course Duration and Prerequisites
• Library enumeration (reaction-based and R-group/Markush) • Diversity selection and clustering, similarity selection • Compound selection optimizing multiple molecular properties simultaneously using Pareto methods • Selection of subset libraries to complement and augment existing libraries • Comparison of libraries	**Onsite Training:** 1 Day **WebEx Training:** 3 Hours **Prerequisites:** Introduction to Discovery Studio

STRUCTURE-BASED DESIGN – DOCKING

This course provides an overview of the Discovery Studio tools used for docking and lead optimization of small molecules into protein targets. The topics include methods used to prepare proteins and ligands for docking, methods to perform different docking methods, methods to perform lead optimization, and methods for scoring, analyzing, refining, and filtering docking results.

Topics	Course Duration and Prerequisites

• Preparation for structure-based design – docking
• Docking methods
• Lead optimization methods
  – Generate analog conformations
  – Free energy perturbation NAMD (prototype)
• Scoring results
• Analysis, refinement, and filtering tools
	Onsite Training: 1 Day
	WebEx Training: 3 Hours
	Prerequisites: Introduction to Discovery Studio

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QSAR

This course is an introduction to the QSAR tools available in Discovery Studio and provides an overview of the various different descriptors that can be calculated within the application. The available QSAR algorithms are described and the main parameters affecting each algorithm are highlighted. Students also receive a comparison of the various techniques.

Topics	Course Duration and Prerequisites
• Introduction to QSAR • Preparing data for QSAR analysis • Working with descriptors • Regression techniques • Modern methods • Example workflow; Applying the generated models	**Onsite Training:** 1 Day **WebEx Training:** 3 Hours **Prerequisites:** Introduction to Discovery Studio

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