TRAINING COURSE CATALOG

BIOVIA DISCOVERY STUDIO
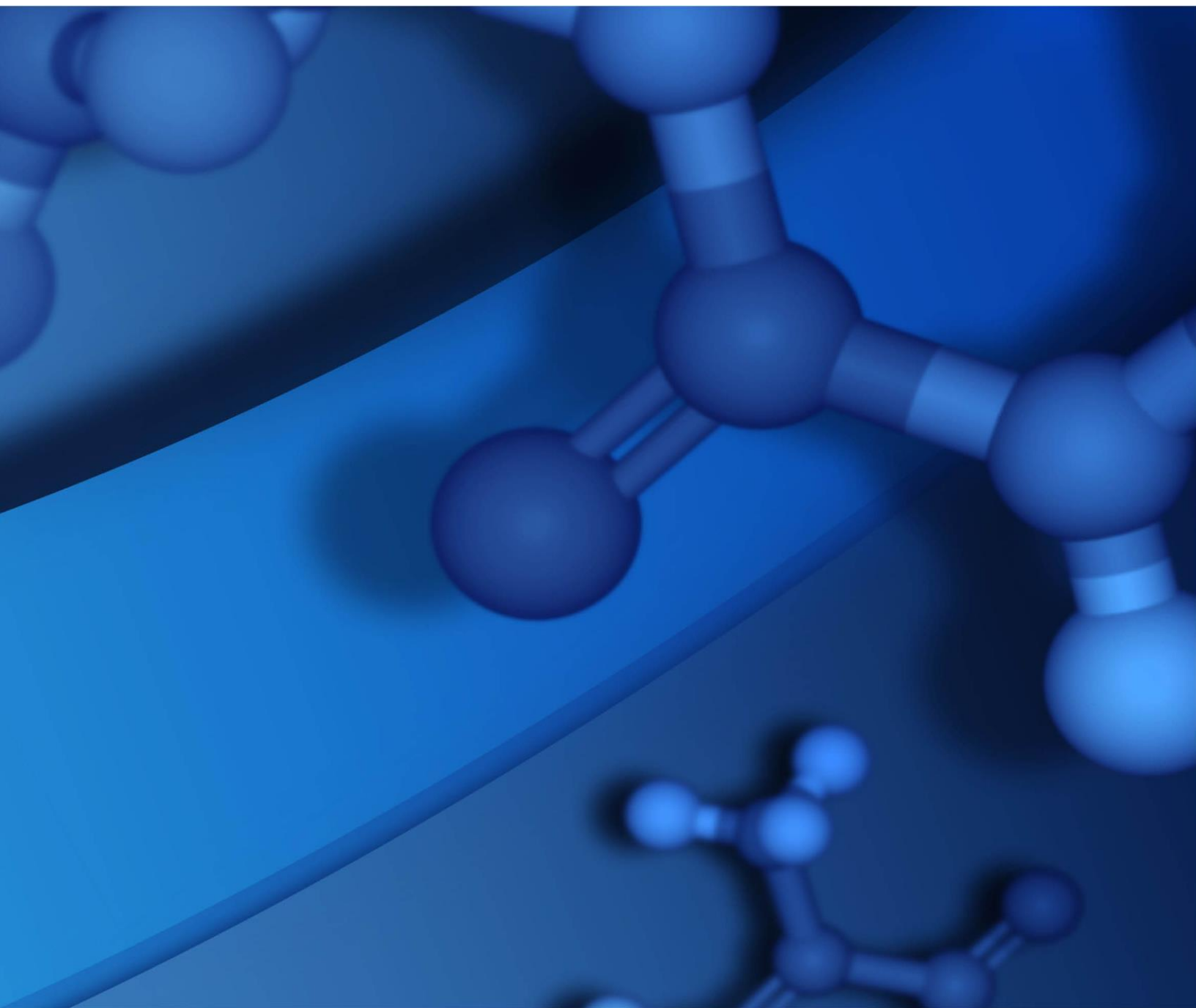
Acknowledgments and References

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Contents

SUMMARY

We are pleased to offer a variety of courses to help you reach productivity quickly and increase the value of your investment in BIOVIA software. A range of training options and delivery methods is available so you can choose a format that best meets your needs. We use structured training materials developed by certified instructional designers and include extensive examples and exercises to maximize practical skills that you can put to use immediately.

Delivery Methods:

- **Instructor-Led Training**: Facilitated by a BIOVIA certified instructor, this training takes place onsite at your location or through a virtual classroom. These courses offer hands-on exercises to enhance the learning experience.

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	Details
- 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 - Customization: Scripting, Toolbars, Tool Sets, Tools Explorer, Tool Panel	**Duration:** 1 Day **Prerequisites:** None **Location:** Onsite or Virtual Classroom

Protein-Based Modeling Courses

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	Details
• The significance, importance, and challenges of performing computational protein-protein docking • ZDOCK and analysis • Refining the poses of RDOCK	**Duration:** 1 Day **Prerequisites:** Introduction to Discovery Studio **Location:** Onsite or Virtual Classroom

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	Details
• 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	**Duration:** 1 Day **Prerequisites:** Introduction to Discovery Studio **Location:** Onsite or Virtual Classroom

Antibody Modeling

This course instructs students in the application of the new Antibody Modeling Cascade. 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	Details
- 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	**Duration:** 1 Day **Prerequisites:** Introduction to Discovery Studio **Location:** Onsite or Virtual Classroom

Simulations

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

Topics	Details
- Energy calculations - Manual and automatic atom potential typing - Energy minimization - Molecular dynamics - Constraints - Solvation models - Trajectory analysis - Force field-based docking - Electrostatic calculations	**Duration:** 1 Day **Prerequisites:** Introduction to Discovery Studio **Location:** Onsite or Virtual Classroom

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	Details
• 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	**Duration:** 1 Day **Prerequisites:** Introduction to Discovery Studio **Location:** Onsite or Virtual Classroom

Ligand-Based Design Courses

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	Details
• Pharmacophore definition and features • Pharmacophore application in drug discovery • Ligand-pharmacophore scoring and mapping • Ligand perception • Conformation generation • Multi-conformer databases	**Duration:** 1 Day **Prerequisites:** Introduction to Discovery Studio **Location:** Onsite or Virtual Classroom

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	Details
- 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	**Duration:** ½ Day **Prerequisites:** Introduction to Discovery Studio, Pharmacophore Modeling in Discovery Studio **Location:** Onsite or Virtual Classroom

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	Details
- 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	**Duration:** ½ Day **Prerequisites:** Introduction to Discovery Studio, Pharmacophore Modeling in Discovery Studio **Location:** Onsite or Virtual Classroom

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	Details
- 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	**Duration:** ½ Day **Prerequisites:** Introduction to Discovery Studio, Pharmacophore Modeling in Discovery Studio **Location:** Onsite or Virtual Classroom

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	Details
- Introduction to Fragment-Based Drug Design - Working with fragments and proteins in Discovery Studio - Preparation (Retrosynthetic Combinatorial Analysis Procedure (ReCAP) approach) - Analysis - Fragment-based drug design modes - REPLACE, GROW, PLACE	**Duration:** 1 Day **Prerequisites:** Introduction to Discovery Studio **Location:** Onsite or Virtual Classroom

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	Details
- 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	**Duration:** 1 Day **Prerequisites:** Introduction to Discovery Studio **Location:** Onsite or Virtual Classroom

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	Details
- 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	**Duration:** 1 Day **Prerequisites:** Introduction to Discovery Studio **Location:** Onsite or Virtual Classroom

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	Details
- Introduction to QSAR - Preparing data for QSAR analysis - Working with descriptors - Regression techniques - Modern methods - Example workflow; Applying the generated models	**Duration:** 1 Day **Prerequisites:** Introduction to Discovery Studio **Location:** Onsite or Virtual Classroom

Advanced Courses

Scripting

Discovery Studio provides a client interface for working with a variety of data. 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	Details
• Introduction to Perl scripting language • 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	**Duration:** 1 Day **Prerequisites:** Introduction to Discovery Studio **Location:** Onsite or Virtual Classroom

Discovery Studio Pipeline Pilot Integration

This course provides an overview of working with the BIOVIA Discovery Studio component collection and provides hands on examples of Discovery Studio protocol customization.

Topics	Details
• 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)	**Duration:** 1 Day **Prerequisites:** Introduction to Discovery Studio **Location:** Onsite or Virtual Classroom