BIOVIA

3DEXPERIENCE®

BIOVIA DRAW

Datasheet

BIOVIA Draw (32 and 64bit) enables scientists to draw and edit complex chemically modified biomolecules (CMBs), molecules and chemical reactions with ease, facilitating the collaborative searching, viewing, communicating and archiving of scientific information.

DASSAULT SYSTEMES

FASTER AND EFFICIENT

BIOVIA Draw brings additional speed and efficiency to chemical structure drawing via the all-purpose drawing tool:

- Continuously draw bonds, pull out rings and add atoms using all-purpose drawing tool
- Drag-and-drop commonly-used structures and chemical abbreviations onto the toolbar for reuse
- Right-click for atom, bond, fragment properties and query options
- Hover over atoms and edit them without right-click

Furthermore, it includes common tasks like:

- Quickly retrace steps using multiple undo/redo
- Easily create structures with R-groups for queries or enumerations
- Annotate reaction schemes with text, color and a variety of arrow styles
- Easily create publication-quality structures for inclusion in Microsoft Office documents and presentations (up to 1200 DPI)

EASY TO INTEGRATE AND CONFIGURE

As an enterprise software application, BIOVIA Draw offers flexible integration with custom Java® and .NET applications as well as integration with BIOVIA Insight and Insight for Excel, BIOVIA Registration, BIOVIA Workbook, BIOVIA Notebook and BIOVIA CISPro. Modify the chemical drawing look-and-feel according to the organization's needs by configuring the applications XML UI.

- Create custom add-ins to enhance the scientist's drawing experience. Such examples include: NMR prediction, create TLC, Enumerate actions
- Integrate with existing desktop applications
- Leverage Web applications for query and browsing

For scientists—Quick and efficient structure and query drawing

- Structure converter converts structure-to-IUPAC name and IUPAC name-to-structure (now including enhanced stereochemistry); structure-to-canonical SMILES and SMILES-to-structure; structure-to-InChI name and InChI name to-structure; and structure-to-InChI key (now includes RInChI for reactions)
- Create structures using the "Structure Resolver", search common structure identifiers like CAS number, name, MDL Number, SMILES, InCHi and more via webservices provided by the following online chemical databases; NCI/CADD (which currently has 96M unique structures), PubChem (116M unique structures), BIOVIA DiscoveryGate Available Chemicals Directory (16M unique structures), or configure others to retrieve the corresponding structure without having to draw it
- Create and edit haptic bonds, Markush bonds (variable attachments), polymers, formulations and mixtures (S-groups)
- Create and edit R-group (Markush) queries including built-in R-group query logic
- Add reagent information to reactions and save this additional information in the reaction file (rxn) along with the reactant and product information
- Create and edit 3D structures
- Create SDFiles from searching SDFiles, molfiles or canvas fragments
- Open SDFiles and view contents, check availability against BIOVIA DiscoveryGate Available Chemicals Directory, calculate properties, search within the open file, export or report on the results and calculations
- Copy as and paste as options:
  - Molfile, Sketch string
  - IUPAC
  - SMILES, InCHi (key or string), NEMA, Chime
  - HELM, Sequence
  - Bitmap, Metafile, Text
- Customize symbols including composite symbols
- Choose from large library of protecting group templates
- Take advantage of improved chemical recognition of tetrahedral and geometric stereogenic centers made possible by BIOVIA NEMA algorithm
- Open ChemDraw CDX files in BIOVIA Draw
- Calculate properties on structures as you draw (AlogP, Polar Surface Area, Hydrogen and Stereo counts, composition, weights and formula)

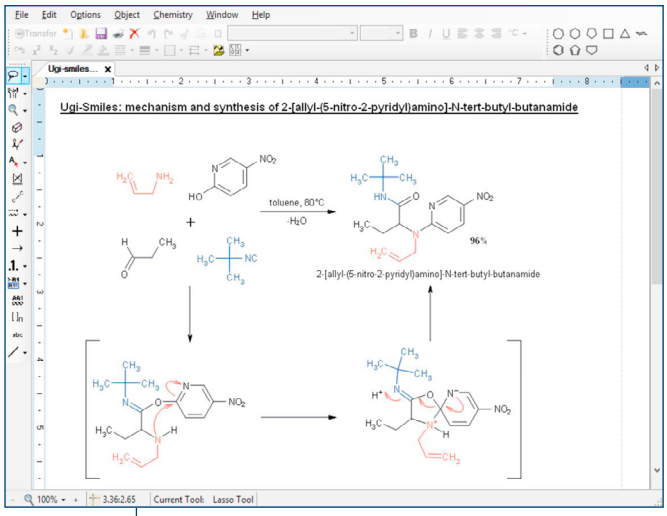


Figure 1: Drawing a synthesis suitable for high-quality printing is simple with BIOVIA Draw. The product name displayed below the structure was generated automatically using the included structure-to-name generator

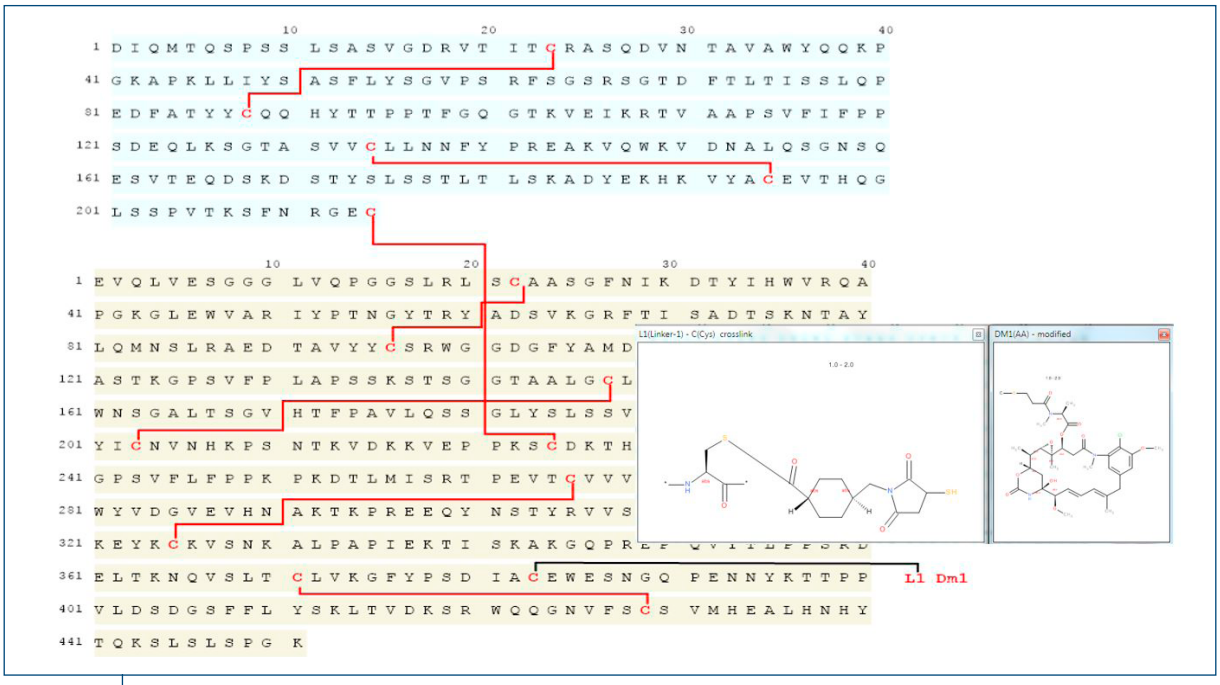


Figure 2: Easily create, register, search and present 1- and 3-letter peptides, biologics, DNA, and RNA. Modify sequences to include unnatural residues, mutations and bridges. Use templates to add HELM monomers, custom residues (Peptide, DNA, RNA), attachments, linkers and protecting groups.

For chemists — Draw, register, search and report on Stereochemistry and Enhanced stereochemistry

- BIOVIA Draw allows scientists to quickly sketch and define the stereochemistry and enhanced stereochemistry (ABS, OR, AND) for:
  - Tetrahedral centers for Carbon, Nitrogen, Sulphur and Phosphorus
  - Axial stereochemistry for
    - Allenes
    - Atropisomers
  - Geometric isomers for cis/trans double bonds
- BIOVIA Draw determines the CIP labels for the chiral area, including meso, pseudo and unknown
- Draw users can choose to display stereo labels and can customize these labels

For biochemists — Draw, register, search and report on chemically modified peptide or nucleotide sequences

- Create 1- and 3 - letter peptide, DNA or RNA sequences with a Sequence tool
- Use the same tool to draw crossing bonds, disulfide bridges and attach side-chain protecting groups
- Build custom nucleic acids using a library of riboses, phosphates and bases
- Import and convert; text, XHELM, HELM, FASTA, Swiss-Prot, PDB and EMBL files into chemically significant sequences
- Expand residues in a sequence to full structure to illustrate chemical modifications
- Launch the BIOVIA Pipette Sketcher or the Pistioia Alliance HELM Editor to generate and edit HELM string notations
- Synchronize automatically with the "Centralized Library", a library of building blocks for CMBs and biologics, which are managed using Pipeline Pilot Chemistry Collection. The library comes with the Pistoia Alliance's set of over 730 monomers and allows customers to add their own items

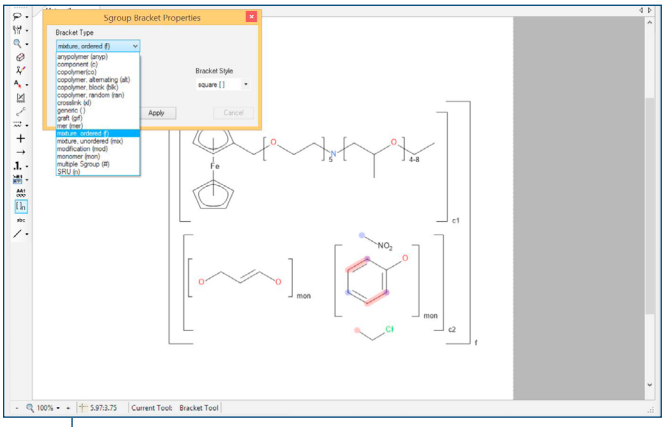


Figure 3: All haptic, polymer, mixture and formulation S-group features are supported. Variable attachments (also known as Markush bonds) also depict where attachments are possible. In this example, a combination of Markush bond, Generic and data S-groups is used to represent a Markush structure.

For developers — Add structure drawing and display to your applications, and customize according to your organizational workflows

- An updated integration to BIOVIA Pipeline Pilot* now enables developers and administrators to provide more extensibility options to BIOVIA Draw utilizing the Pipeline Pilot Collections such as Chemistry*, ADMET* etc. which provides support for different types of outputs
    - Calculated Values
    - Molecules
    - SD Files
    - Charts and Tables
- Users can run example or custom protocols (once published) on their structures from within BIOVIA Draw and choose which parameters are needed to provide the answers they need
- Use the "BIOVIA Draw Bridge" to render and edit in Google Chrome®, Microsoft Edge® browsers or Java/JavaScript custom built applications.

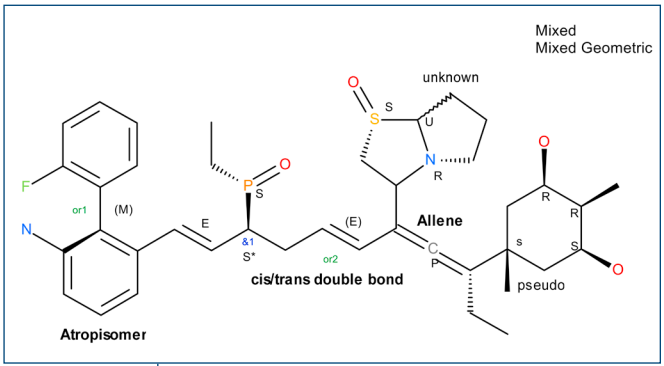


Figure 4. Comprehensive stereo and enhanced stereochemistry support.

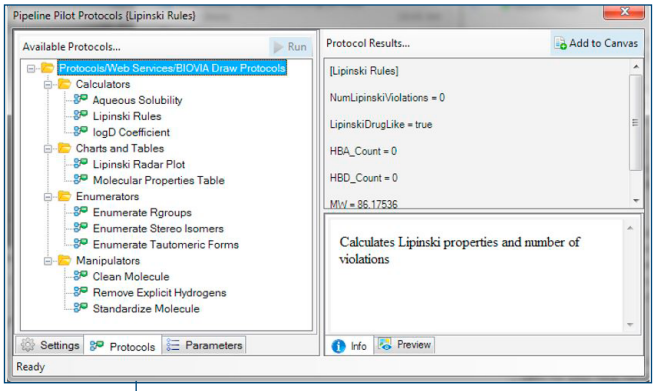


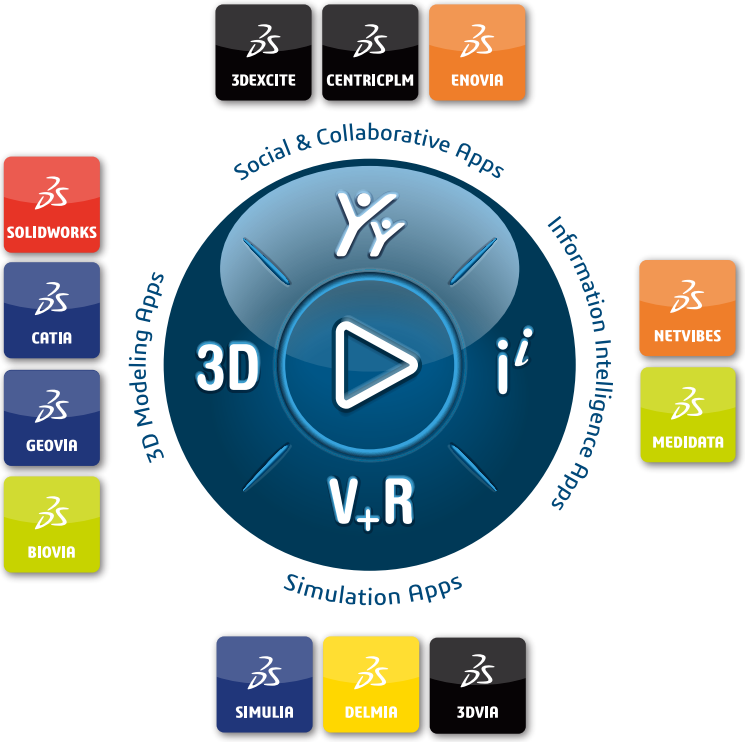
Figure 5: Pipeline Pilot integration in Draw provides users the ability to perform additional functions. Included in Draw are example protocols they can run against structures of interest

- BIOVIA Draw supports Microsoft Windows 10, 11 (32 and 64bit) and Office 2019, 2021 (32 and 64bit) software
- Easily extend BIOVIA Draw's capabilities with custom add-ins, including:
    - ACD/Labs calculators*
    - ACD/Labs Name*
    - Bio-availability (Rule of 5)
    - R-group/S-group/stereochemistry/reaction enumerators
    - OSRA
    - Create TLC
    - Many predictive Spectra and look abilities available

*separate license required

Please contact BIOVIA support or visit the BIOVIA Drug Discovery & Development Community center / Wiki pages < BIOVIA Draw Add-ins for information on available add-ins

LEARN MORE



Our **3D**EXPERIENCE® platform powers our brand applications, serving 11 industries, and provides a rich portfolio of industry solution experiences.

Dassault Systèmes, the **3D**EXPERIENCE Company, is a catalyst for human progress. We provide business and people with collaborative virtual environments to imagine sustainable innovations. By creating 'virtual experience twins' of the real world with our **3D**EXPERIENCE platform and applications, our customers push the boundaries of innovation, learning and production.

Dassault Systèmes' 20,000 employees are bringing value to more than 270,000 customers of all sizes, in all industries, in more than 140 countries. For more information, visit **www.3ds.com**.

Europe/Middle East/Africa
Dassault Systèmes
10, rue Marcel Dassault
CS 40501
78946 Vélizy-Villacoublay Cedex
France

Asia-Pacific
Dassault Systèmes K.K.
ThinkPark Tower
2-1-1 Osaki, Shinagawa-ku,
Tokyo 141-6020
Japan

Americas
Dassault Systèmes
175 Wyman Street
Waltham, Massachusetts
02451-1223
USA

DASSAULT SYSTEMES | The **3D**EXPERIENCE® Company