BIOVIA DRAW
Datasheet

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

FASTER AND MORE EFFICIENT

BIOVIA Draw has the same look-and-feel as ISIS/ Draw, but brings additional speed and efficiency to chemical structure drawing:

- 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
- Quickly retrace steps using Multiple Undo/Redo
- Easily create structures with Rgroups 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
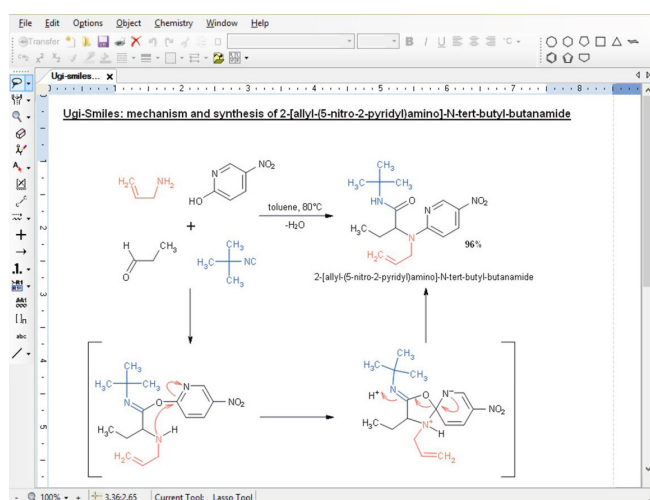

Figure 1: Drawing a synthesis suitable for high-quality printing is simple with BIOVIA Draw. The product name displayed below the structure was generated automatically using the included structure-to-name generator.

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, Accelrys Isentris® and ISIS applications. Modify the chemical drawing look-and-feel according to the organization's needs by configuring the applications XML.

- Create custom add-ins to enhance the scientist's drawing experience
- 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 nameto-structure; and structure-to-InChI key
- Create structures using the "Structure Resolver", search common structure identifiers like CAS number, name, MDL Number, SMILES, InChi and more via webservice provided by the following online chemical databases; NCI/CADD (which currently has 96M unique structures), PubChem (63M unique structures), Chemspider (36M unique structures), BIOVIA DiscoveryGate ® Available Chemicals Directory (13M unique structures), or configure others to retrieve the corresponding structure without having to draw it
- Create and edit haptic bonds, polymers, formulations and mixtures (Sgroups)
- Create and edit Rgroup (Markush) queries including built-in Rgroup query logic
- Create and edit 3D queries, all 3D query features supported including 3D rotate
- Create SDFiles from 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
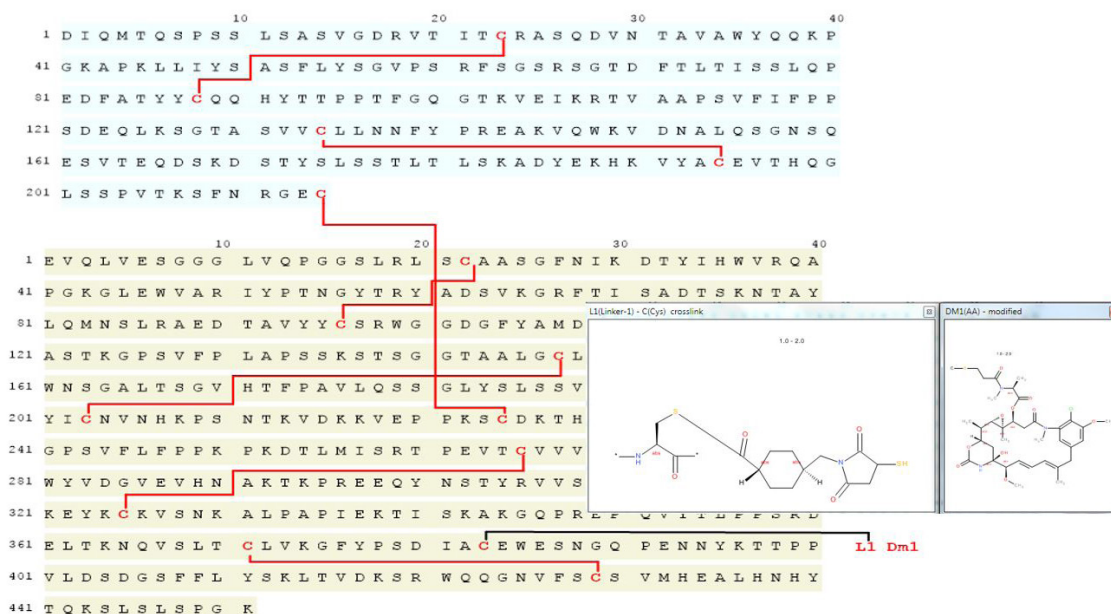   - HELM, Sequence
    - Bitmap, Metafile, text

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.

- 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
- Create and edit ISIS-compatible sketches, edit legacy sketches with improved cleaning of sketches
- Ease the transition with familiar ISIS/Draw-like chemical drawing tools and behaviors
- 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 3: All haptic, polymer, mixture and formulation Sgroup 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 Sgroups is used to represent a Markush structure.

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
- 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 HELM Editor to generate and edit HELM string notations

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 BIOVIA Draw in Microsoft Internet Explorer® browser
- BIOVIA Draw supports Microsoft Windows 7, 8.1 (32 and 64bit) and Office 2010, 2013 (32 and 64bit) software
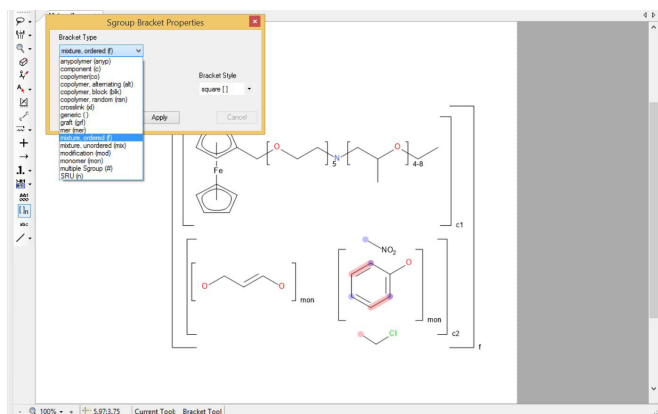
- Easily extend the BIOVIA Draw look-and-feel with custom addins, including:
  - ACD/Labs calculators*
  - ACD/Name*
  - Bio-availability (Rule of 5)
  - RGroup/SGroup/Stereochemistry/Reaction Enumerators
  - OSRA
  - Create TLC
  - Many predictive Spectra and look abilities available

Please contact BIOVIA support or visit the Community center for information on available addins
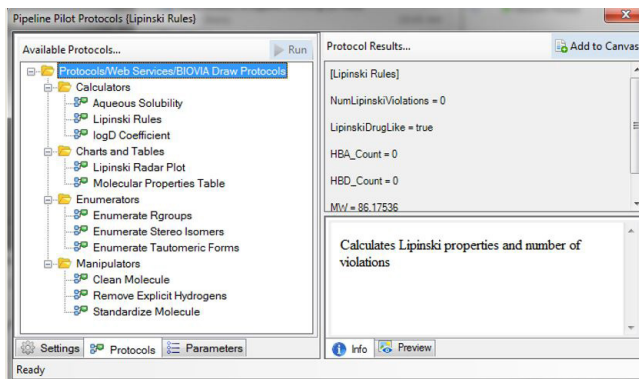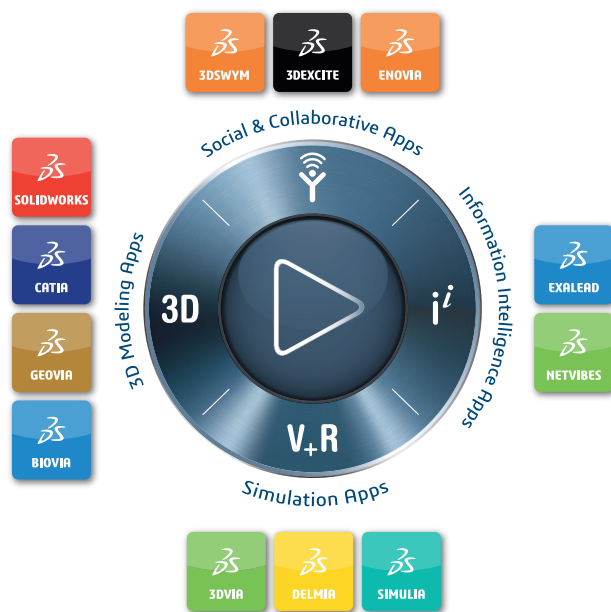
*separate license required

Figure 4: 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

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