accelrys®

ACCELRYS DRAW 4.1

Release Notes

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Contents

About this Document

This document contains instructions and notes for Accelrys Draw 4.1. This release includes defect fixes and known issues for the current release of Accelrys Draw 4.1.

Accelrys® Draw enables scientists to draw and edit complex molecules and chemical reactions with ease, facilitating the collaborative searching, viewing, communicating, and archiving of scientific information.

Note: Accelrys JDraw Applet for drawing and rendering in web applications is available at no charge to Accelrys Draw Enterprise Edition licensees as well as to academic and non-profit institutions. For additional information, see http://accelrys.com/products/informatics/cheminformatics/draw/jdraw.php.

Faster and More Efficient

Accelrys 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
- 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

Easy to Integrate and Configure

As an enterprise software application, Accelrys Draw offers flexible integration with custom Java® and .NET® applications as well as integration with Accelrys Isentris® and ISIS® applications. Use XML to configure the chemical drawing look-and-feel according to the organization's needs.

- 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; structure-to-canonical SMILES and SMILES-to-structure; structure-to-InChI name and InChI name-to-structure; and structure-to-InChI key; and structure-to-NEMA key.
- 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
- Calculate-As-You-Draw
- Create and edit 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
- 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 NEMA algorithm

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
- Convert text from the clipboard, FASTA, Swiss-Prot, PDB, and EMBL files into chemically significant sequences
- Expand residues in a sequence to full structure to illustrate chemical modifications
- Create an opposite sense sequence from an existing sequence in one step
- Create feature chains with a Sequence Create Chain tool – features can be overlapped and highlighted in different colors
- The sequence is saved in the SCSR molfile format by default that is compact but keeps full chemistry (Please see SCSR paper for detail - J. Chem. Inf. Model. 2011, 51, 2186–2208).

For Developers - Add Structure Drawing and Display to your Applications, and Customize According to your Organizational Workflows

Use Accelrys Draw in Microsoft Internet Explorer® browser

- Accelrys Draw supports Microsoft Vista, Windows 7 and Office 2003/2007/2010 software. For a complete listing of hardware and software requirements read the *Accelrys Draw 4.1 System Requirements* document.
- Easily extend the AccelrysDraw look-and-feel with custom add-ins, including:
- 2D-to-3D Structure Converter
- ACD/Labs calculators*
- ACD/Name*
- Bio-availability
- Isotopomer Distribution
- Enumerator

*Separate license required.

System Requirements

The system requirements for Accelrys Draw 4.1 are detailed in the *Accelrys Draw 4.1 System Requirements* document. This file is included in the Accelrys Draw 4.1 documentation zip file. The zip file is located on the Accelrys Community web site. If you are unable to locate the System Requirements document, contact Accelrys Customer Support at support@accelrys.com or support-japan@accelrys.com (for customers in Japan).

Redirect Policy

Accelrys Draw 4.1 ships with redirects from:

- Symyx Draw 3.2
- Symyx Draw 3.3
- Accelrys Draw 4.0 (any version including Service pack and special releases)
- Any previous versions of Draw 4.1, for example an Alpha or Beta

All redirections point to the current version of Accelrys Draw 4.1. The redirect policy also applies to the published API. Some of the exposed APIs are not documented and are subject to change. It is highly recommended, however, that only the published APIs be used. If you are using any of the non-documented APIs, please contact Customer Support and inform us which non-documented APIs you are using so that we can reduce the chances that changes will affect your applications.

Getting Help

An updated version of the Release Notes might be available at the Accelrys Community site. To locate the updated Release Notes for this product:

1. Go to the Accelrys Community site for Accelrys® Draw: https://community.accelrys.com/community/accelrys_direct__draw__and_jdraw
2. Locate, and download the documentation for this version of Accelrys Draw 4.0 Service Pack 1 (SP1).

If you have any questions, please contact Accelrys Customer Support at:

- Support for Accelrys Products is available at support@accelrys.com or support-japan@accelrys.com (for our customers in Japan).
- Accelrys Support on the Web: https://community.accelrys.com/index.jspa

A complete list of regional Accelrys Customer Support offices is available at:

- Accelrys Support Offices: http://accelrys.com/customer-support/contact.html

What's New

This release of Accelrys Draw 4.1 includes the following new features and enhancements.

New features in Accelrys Draw 4.1

The following are illustrated in more detail in the end-user Help.

- Sequence Create Chain tool allows you to specify Type, Name, Color, and whether the chain is discontinuous (breaking).
- The Sequence Create Chain tool allows you to create overlapping chains.
- Attachments toolbar appears on DNA and RNA tools, as well as on the AA toolbar.
- Linker toolbar is added to the sequence template management tools.
- Zero order bond properties can be assigned to a bond and you can set zero order bond display preferences.
- Hydrogen bond tool has been added and can be used to lock sequences.
- Dative/coordination bond tool has been added.
- Variable attachment bond (Markush bond tool) has been added to allow you to define a set of atoms, any one of which might be the attachment point. Configurable Markush colors and Markush attachment point shape.
- Atom list query feature can be combined with a variable attachment bond and is supported in polymers.
- Variable attachment bond supports up to 4 independently attached groups, and up to 10 dependently attached groups. Variable attachment bond supports single, double, and triple bonds, as well as formula and formula weight calculation.
- Haptic bond tool facilitates drawing metallocenes and Options > Settings > Haptic/Markush structure > Haptic bond style > Dotted line displays differently from Bonds > Aromatic bonds as circle
- Chemistry > Discovery Studio Visualizer integration allows you to see a 3D depiction of the currently selected structure.
- DNA/RNA sequences have options to change sequence direction, convert sense to anti-sense (or anti-sense to sense), or add an opposite sense sequence.
- Bio Objects templates support having multiple active toolbars.
- Variable repeat groups can be single integer or variable count (for queries), including a range and non-consecutive numbers.
- New option to show sequence cyclic bond.
- Custom sequence template is supported. You can also customize other Types, such as Attachments and Linkers. This allows the user to draw new types of sequences.

The Deployment Guide (a PDF document distributed in the same location as the System Requirements) explains two new types of deployment (in addition to the standard MSI and silent installation):

- ClickOnce, introduced in Draw 4.1 for *enterprise-level* ease-of-deployment. Please see the installation guide for more details.
- Portable deployment (without an installer, for any file system, including a thumb drive). Please note that this version does not support OLE (i.e. Microsoft office inter-operability through copy/paste/double-click). Please see the installation guide for more details.

Fixed Defects

This release includes the following fixed defects:

Defect #	Priority	Description
DRAW-3988	High	relative paths in Draw configuration files
DRAW-3942	High	extra bond when deleting brackets via the DELETE button
DRAW-3687	High	At German Regional Settings bonds length of cleaned structure becomes 1,27 cm instead of standard value
DRAW-3072	High	All-purpose tool should use multi-bond tool again
DRAW-3941	High	bug reports - how to turn them off?
DRAW-3033	High	Relative coordinates transformed to Absolute coordinates
DRAW-1764	High	Cheshire Action as a button on the toolbar?
DRAW-1723	High	Request include Ornithine as a standard template Amino Acid
DRAW-1689	High	Problem with Clean Reaction
DRAW-1678	High	Grouping with No_Structure
DRAW-1674	High	0 termination of right leaving group issue
DRAW-1656	High	Custom residues with 3-letter codes
DRAW-1611	High	How to modify the resolution of Draw image generation?
DRAW-11548	High	Undo after deleting a sequence makes H:s sprout out from the residues
DRAW-11545	High	Residue left when deleting a modified sequence
DRAW-11544	High	it's not possible to delete residues with the delete key
DRAW-11542	High	Deleting residues can result in an exception
DRAW-11487	High	Hydrogens visible despite setting for hydrogen labels is "Off"
DRAW-11059	High	Set format of sequence that is put on the clipboard
DRAW-10960	High	ppt OLE displays other structure than what is contained
DRAW-4009	Medium	unable to grab bond with short standard bond length settings
DRAW-3983	Medium	Documentation: Beilstein Generic Groups in Draw
DRAW-3974	Medium	Drawing chains of atoms through only keyboard shortcuts fails with Accelrys Draw.
DRAW-3943	Medium	powerpoint and Symyx Draw
DRAW-3896	Medium	Symyx Draw 4.0 : amino acids problem
DRAW-3885	Medium	Hydride (H-) shows up as (HH2-) when Show Hydrogen Labels is set to Hetero

DRAW-3863	Medium	Renditor throws an error if used on a form that's invoked by calling Form.ShowDialog()
DRAW-11265	Medium	Trying to add Accelrys Draw to CambridgeSoft ELN and getting odd structures for multiple groups
DRAW-11237	Medium	Renderer does not show repeating units numbers if the X-coordinate is negative on the bracket
DRAW-11539	Medium	Residues remains when sequence is deleted
DRAW-11471	Medium	Bad layout when expanding a cyclic di-peptide
DRAW-11467	Medium	Incorrect sketch file saved in Draw 4.0 SP1
DRAW-11367	Medium	Draw installer skips installation of .Net Framework 2 if Framework 4 is already installed
DRAW-11360	Medium	Additional Substituents menu item shown in Help is missing
DRAW-11541	Medium	No indication that a residue was modified
DRAW-11225	Low	Link to Draw Interactive Videos in Help Browser is broken - 404 Page not Found error

Known Issues

This release of Accelrys Draw 4.1 includes the following known issues:

IMPORTANT! Biologics that use the new Self-Contained Sequence Representation (SCSR) representation are written in an enhanced molfile (.mol) format available in Accelrys Draw 4.0, might not be understood by other chemistry software packages, or earlier versions of MDL/Symyx Draw. If you require a compatible format, export the structure in a format that is understood by the software. Note, the enhanced molfile (.mol) format is **NOT** backwards compatible.

Defect #	Severity	Description
DRAW-11190	High	OLE in Word gets huge after modification and retransfer into Word **Workaround:** The corner of the OLE object in Word can be dragged in order to properly resize it.
DRAW-11285	Medium	Laptop does not shut down until Accelrys Draw is killed On XP computers with some graphics cards problems can be observed shutting down the machine after Draw was used for working with MS Office documents. This has been reported with NVIDIA graphics cards (e.g. Quadro FX 360M or FX Go1400). Manual killing of the Draw process via taskmanager resolves the problem. **Workaround:** Disabling of the graphics hardware acceleration: 1. Right-mouse click on the Desktop and select Properties 2. Go to Settings > Advanced > Troubleshoot 3. Set the Hardware Acceleration Level from Full to None.
327548	High	The **Editor Selection** switch in the **Tools** menu of ISIS for Excel is inactive, if ISIS/Draw is selected as the default editor during installation of Symyx Draw. In this case ISIS/Draw is called by ISIS for Excel independent of how the switch is set. With Symyx Draw as the default editor the switch is fully functional.
DRAW-1684	High	Chemical brackets are lost after Set to R/Set to S action **Workaround:** Set **Show Stereoconfiguration** to **On** and use the appropriate stereobond tool to adjust the stereogenic center's parity.
328959	High	The saving/reopening of sequences in rxn file is incorrect. **Note:** Reactions with sequences are not supported with Accelrys Draw 4.1.
327481	Medium	By default, on 64-bit machines, Accelrys Draw 4.1 installs into `C:\Program Files(x86)\Accelrys\Accelrys Draw 4.1`. With an installation of ISIS/Base on the same machine, the path in **Options**>**Structure Editor**>**Symyx Draw** --- Choose Draw Application dialog must be manually edited to display the path: `C:\Program Files(x86)\Accelrys\Accelrys Draw 4.1`

328852	Medium	Pasting structures into Outlook 2007 results in crash or exception **Workaround:** "paste special" and insert as MDL.Draw.Object. Please note: this problem only applies to emails in *edit mode*. Incoming emails with Outlook 2007 or 2010 are generally read-only and editing of inline structures by double-click is not possible. These structures can be copied into Accelrys Draw. Structures sent with Outlook 2010 come in as images. Please note: Outlook 2010 by default composes HTML emails which generally can't contain OLE objects, e.g. live chemical structures. To be able to send such structures emails have to be composed in RTF format like with prior version of Outlook.
328981/ 328984	High	Sequences created before Draw 4 cannot reliably be edited (or copied) in **Sequence View**. They must be handled as legacy structures in **Structure View**. In a future release we will include a converter that enables **Sequence View** edits.
329025	Medium	Modification (of Edit Residue) is lost if a new Draw tab is opened before the changes are saved **Note:** It is necessary to complete an edit residue task before starting a new tab for more editing.
DRAW-11524	Medium	v3000 molfile with sgroup empty field value that is not the last one fails to read correctly.
DRAW-11498	Medium	Charge on haptic bonded metal not suppressed if it contains other ligands.
DRAW-11249	Medium	After a "modify" installation, doc folder, examples and tools folder are missing. These are the elements that are additionally installed when "developer" mode is selected during installation.
DRAW-11401	Medium	Linker Attachment name display reversed on attaching to left end label with N-residue.
DRAW-11400	Medium	Linkers structures gets pasted over the sequence when there is no attachment point to link to. **Workaround:** undo the pasting operation
DRAW-11398	Medium	Single sequence label when saved as mol file and reopened appears as 3 letter code in sequence view.
DRAW-11394	Medium	Custom Periodic table and Cheshire Action Examples link are not working under Examples folder of Draw 4.1. **Workaround:** Go to Start>All Programs>Accelrys> Accelrys Draw 4.1>Examples and click on Custom Periodic table. Observed started batch file disappears and Accelrys Draw 4.1 not gets launched. This issue is because path location in batch file is incorrect ""C:\Program Files\Accelrys\Accelrys Draw 4.1\SymyxDraw.exe" PTableDemo.xml" instead of Symyx it should be Accelrys.

DRAW-10978	Low	ISIS Base crashed when rerun the standalone installer from Add-Remove control panel for changing the editor.
DRAW-3818	High	Draw crashes at cut mol structure having multiple SGroup as RGroup member. **Workaround:** copy and paste in a new tab, and close the original tab - do not delete, cut, or use cntrl-X.
DRAW-11463		No prompt for attachment point when creating a bond from K to Y The automatic linking is designed to carry out a condensation reaction so water is eliminated. If alternative bonding is needed it must be manually entered by editing the structure.
DRAW-11419		When a variable attachment is extended the extension is not incluced in the selection resulting from a cntrl+Click **Workaround:** If the terminal group of a variable attachment entity is extended cntrl-select and molecule select may not include the new added pieces. Use lasso -select in this case. We recommend that the substructure be drawn before the variable attachment bond. When the the variable attachment bond is dragged out terminate it at the attachment point in the substructure. This will include the entry unit in any selection process. Note that if the substructure is subsequently edited, the new parts may not automatically be incorporated during the molecule-select or cntrl-select operations.
DRAW-11417		Draw does not recognize biphenyl, or biaryl stereo centers. If you try to set Stereoconfiguration on a biaryl stereocenter, you wil get the message “Highlighted atoms are not stereo centers.”
DRAW-11366		OLE Sequence object from MS Word doesn't appear in Draw if wrap length is changed from the default value Any reversed sequence will not be realigned by wrap length/ block size change. We are aware of this issue and will address it in a future release.

IMPORTANT! In cases where Accelrys Draw 4.1 EE is installed in combination with other Accelrys client applications like Isentris, Logistics or Accelrys Notebook which include prior embedded versions of Accelrys Draw, un-installation of Accelrys Draw 4.1 EE may not result in a working setup of that prior version. In that case a repair installation of the respective client application will become necessary.

ISIS/Base and ISIS for Excel (IFE) Editor Switches

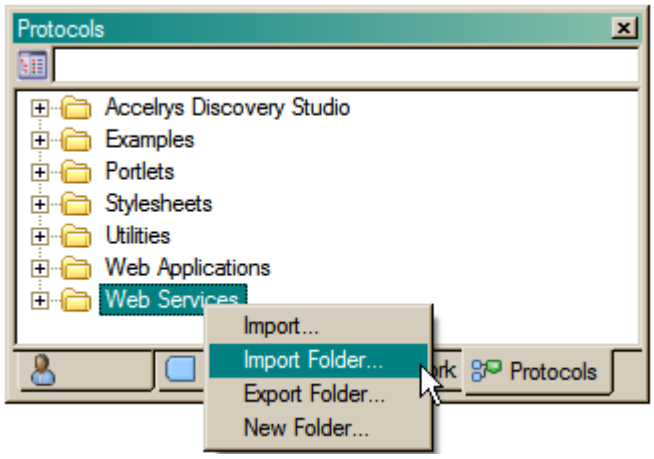
To ensure ISIS/Base and IFE display switches to give the end-user the choice between using ISIS/Draw or Accelrys Draw as the editor launched with the mentioned products, make sure to install Accelrys Draw 4.1 after installing ISIS/Base or IFE.

If you need assistance installing the software, or if you have any defects to report or feature requests, please contact us by email at support@accelrys.com or support-japan@accelrys.com for our customers in Japan.

Importing the Draw Pipeline Pilot Calculators protocols into Pipeline Pilot 8.0

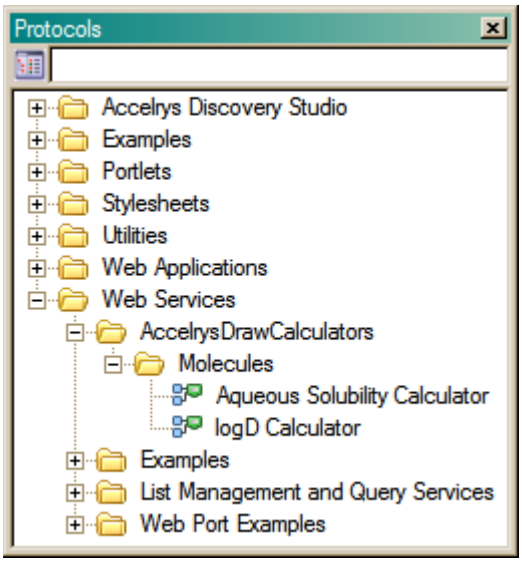
Draw allows you to connect to Pipeline Pilot 8.0 (or higher) to utilize Draw Pipeline Pilot calculators. The **Draw Pipeline Pilot Calculator** feature allows you to calculate the **aqueous solubility**, or **logD** of a structure or molecule on the drawing canvas. You must have Accelrys Pipeline Pilot 8.0 (or higher) installed, and have its web service properly configured for this functionality to be available.

1. Install Pipeline Pilot 8.0 (or higher).
2. Start Pipeline Pilot 8.0 (or higher).
3. On the **View** menu, point to **Explorer Windows**, and then click **Protocols**.
4. Right-click the **Web Services** folder and then click **Import Folder…**.



Pipeline Pilot 8.0 protocols dialog

5. Navigate to `<root folder>\Program Files\Accelrys\Accelrys Draw 4.1\Pipeline Pilot`, and select the **AccelryDrawCalculators** folder.
6. Click **OK** to confirm your selection and close the dialog box, or click **Cancel** to discard your selection and close the dialog box. In Pipeline Pilot, the **Protocols** > **Web Services** folder now contains a folder called **AccelrysDrawCalculators**, and a respective sub-folder called **Molecules**. In the **Molecules** folder are the **Aqueous Solubility Calculator** and **logD Calculator** protocols.



Pipeline Pilot 8.0 protocols dialog

7. Close Pipeline Pilot 8.0 (or higher).

To use the **Draw Pipeline Pilot Calculator**, or configure the Pipeline Pilot web services in Draw, see the topic *Pipeline Pilot Calculator* in the Draw end-user online help.

If you encounter any errors during the Draw Pipeline Pilot Calculators import, or during the Pipeline Pilot web services configuration, then contact your Draw administrator, or contact Accelrys Customer Support.

Previewing a Thumbnail of a Chemical Structure File Using the Windows File Explorer

This feature allows you to preview a thumbnail of a chemical structure file within the **Windows File Explorer** and the file dialog (for example, **Save** and **Load**). This feature operates on molfiles (.mol), rxnfiles (.rxn), sketch (.skc) files, and CDX (.cdx) files. During the installation of Accelrys Draw, you are prompted to select whether to allow the preview of thumbnails of chemical structure files.

Note: This feature is not available in 64-bit platforms.

To Preview a Thumbnail of a Chemical Structure File in Windows Vista or Windows 7:

1. Click the **Start Menu**.
2. Click **Control Panel** > **Folder Options** > click the **View** tab. Under **Advanced Settings** > **Files and Folders**, turn off the **Always Show Icons**, **Never Thumbnails** option, and then click **OK**.
3. **(Optional)** In the Explorer window, click **Organize** > **Folder and Search Options**, click the **View** tab > click **Apply to All Folders**, and then click **OK**.

Note: If a chemical structure is large or complex, the thumbnail preview may be slow.

Configuring Citrix to Properly Paste Chemical Structures

Using Citrix-hosted structure editors, chemical structures are pasted as images without structure data. To resolve this problem, Citrix can be configured to properly paste chemical structures.

To configure the Citrix server to include additional clipboard formats:

1. On the Citrix server computer, open the registry editor. Choose **Start** > **Run**. Type **regedit** and click **OK**. The Registry Editor opens.
2. In the Registry Editor:
   - Expand to:

```
HKEY_LOCAL_MACHINE\SYSTEM\CurrentControlSet\Control\Citrix\wfshell\Virtual
Clipboard\Additional Formats
```

   - Add the subkeys `MDLCT`, `MDLSK`, and `ChemDraw Interchange Format` to the **Additional Formats** key.
   - Add to each subkey a new string value "`Name`" and set the value to the name of the subkey.

Intellectual Property

Accelrys Draw™

Accelrys JDraw™

OpenEye™

IUPAC™

Microsoft Internet Explorer™

Firefox™

CambridgeSoft™

ChemDraw™