Accelrys® JDraw

Version 1.1 Service Pack 2 (SP2)

Release Notes

December 7, 2010

CONTENTS

1. Introduction

Accelrys® JDraw is a compact, thin-client, cross-browser applet which enables scientists to edit and render chemical structures.

Accelrys® JDraw 1.1 SP2 includes the following key features:

- Loads quickly in web based applications.

- Provides access to Accelrys's best in class chemical representation.

- Includes components that can use Accelrys's query features to refine hit sets.

- Can be used as a full editor and renderer, or in a render only mode.

- Allows editing of structure in the web-page; you do not have to wait for a separate editing application to start up.

- Supports Clipboard operations with major chemical structure drawing applications, including Accelrys Draw, ISIS/Draw, and ChemDraw.

- Has a familiar look-and-feel that allows Accelrys Draw and ISIS/Draw users to immediately use the functionality without dedicated training.

- Does not require installation; deployment on web server as JAR files that a customer-developer can include in a Java applet or Java application. The Accelrys JDraw components might be used for various purposes, such as allowing end-user chemists to draw query structures, or allowing a result set of structures to display in a grid.

- Provides examples that show:
  - ➢ How to use JavaScript when including the Accelrys JDraw editor in an applet, and how an applet can render multiple structures in a grid.
  - ➢ How a Java application can include the Accelrys JDraw editor, and how a Java application can render multiple structures in a grid.

- Includes an API Reference (javadoc).

- Enhancements to support Sgroups (polymers, mixtures, and formulations) are planned for a future release.

2. JDraw Requirements

For a complete listing of the applet requirements for **Accelrys® JDraw 1.1 SP2**, read the **Accelrys® JDraw 1.1 SP2 System Requirements** document.

IMPORTANT: Accelrys® JDraw Applet 1.1 SP2 might not work with JRE versions prior to those stated in the **Accelrys® JDraw 1.1 SP2 System Requirements** document. In particular, the applet will not work with version **1.6.0.15** due to a defect in the Sun JRE.

3. Getting Help

An updated version of the Release Notes might be available at the Symyx Support site.

To locate the updated Release Notes for this product:

1. Go to the Symyx download site: http://www.symyx.com/downloads/

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2. Log in with your Web site Documentation or Download user account username/password.

3. Choose **Support > Knowledge Base**.

4. To locate the Release Notes, choose the appropriate product name from the drop-down list.

If you need assistance installing the software, or if you have any defects to report or feature requests, please contact Accelrys Customer Support at:

- Support for "classic" Accelrys Products is available at support@accelrys.com or supportjapan@accelrys.com (for our customers in Japan).
- Support for "classic" Symyx Products is available at support@symyx.com or jsupp@symyx.com (for our customers in Japan).
- Accelrys Support on the Web: https://community.accelrys.com/index.jspa
- Symyx Support on the Web: http://www.symyx.com/support

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

- Accelrys Support Offices: http://accelrys.com/customer-support/contact.html
- Symyx Support Offices: http://www.symyx.com/support/contact/worldwide.jsp

4. What's New

This release includes the following new features and enhancements:

4.1 New Features in Accelrys® JDraw 1.1 SP2

- Colored atom labels

- Atom label toolbar

- Extended support of enhanced stereochemistry (V3000)

- R-Group query tutorial

4.2 Enhancements for Accelrys® JDraw 1.1 SP2

User Story / Defect #	Description
US3673	`getMolStringUNIX()` and `getMolStringDOS()` methods for JDraw classes
US5607	Increase whitespace around atom labels

5. Fixed Defects

This release includes the following defect fixes:

Defect #	Severity	Description
DE9917	Crash/Data Loss	Exception appears after Atom-Atom mapping/Undo for N and P atoms in case of Accelrys Draw rxnfile
DE10321	Crash/Data Loss	No assignment of charges possible above +1
DE11948	Major Problem	OnStructureChangedJS event

DE7708	Minor Problem	JDraw bug with continuation character (-) in molfile
DE9535	Minor Problem	HTTPD error log entries due to calls to classes that are not in the jars

6. Known Issues

There are no known issues in this release.

Note: The addition of the new Atom toolbar may cause the applet window to cut-off other areas of the user interface. If you experience this problem, re-size your browser window.

7. Appendix 1

7.1 Use of Linefeeds in Applet Parameter Strings

There is a defect in JRE1.6.0_19 that strips linefeeds away in applet parameter strings (and only there). Because of this, in JDraw 1.1 SP2 we have adopted a convention that when you pass a molfile as an applet parameter in an html file, you should use \n to represent carriage returns. The applet then substitutes the \n for a real carriage return to restore the correct molfile string.

Note that the \n in the mol string is needed ONLY if you are passing a molfile as an applet parameter in an html file. You do NOT need it if you are injecting mol files into an applet via javascript.

Here is an example of a molstring parameter using &#10 which is the ASCII 10 (carriage return).

This will NOT work because the carriage return is stripped by the JRE on arrival and the applet will receive one long line which it is not able to parse.

```
<param name="molString" value="!&#10;  SMMXDraw03261012542D&#10;&#10;  5  4  0  0  0
  0  0  0  0  0999 V2000&#10;    8.4124   -8.4156    0.0000 N   0  0  0  0  0  0  0
  0  0  0  0&#10;    8.4124   -7.5888    0.0000 C   0  0  1  0  0  0  0  0  0  0  0
  0&#10;    9.2182   -7.3054    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0&#10;
  9.2182   -6.4558    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0&#10;    7.7075   -
  7.1094    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0&#10;  2  5  1  6  0  0
  0&#10;  3  4  2  0  0  0  0&#10;  2  3  1  0  0  0  0&#10;  1  2  1  0  0  0  0&#10;M
  END&#10;">
```

Now substitute the &#10 with \n as shown below and everything will work as expected:

```
<param name="molString" value="!\n  SMMXDraw03261012542D\n\n  5  4  0  0  0  0  0  0
  0  0999 V2000\n    8.4124   -8.4156    0.0000 N   0  0  0  0  0  0  0  0  0  0  0
  0\n    8.4124   -7.5888    0.0000 C   0  0  1  0  0  0  0  0  0  0  0  0\n    9.2182
  -7.3054    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0\n    9.2182   -6.4558
  0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0\n    7.7075   -7.1094    0.0000 C   0
  0  0  0  0  0  0  0  0  0  0  0\n  2  5  1  6  0  0  0\n  3  4  2  0  0  0  0\n  2  3
  1  0  0  0  0\n  1  2  1  0  0  0  0\nM  END\n">
```

8. Intellectual Property

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