

Getting started with **Bioclipse 2.6**

This is a short introduction to help you get started with Bioclipse 2.6. The first part deals with downloading and installing Bioclipse, which looks a bit different depending on your operating system. Here we describe Windows 7, Mac OS X and Ubuntu Linux. Happy Bioclipsing!

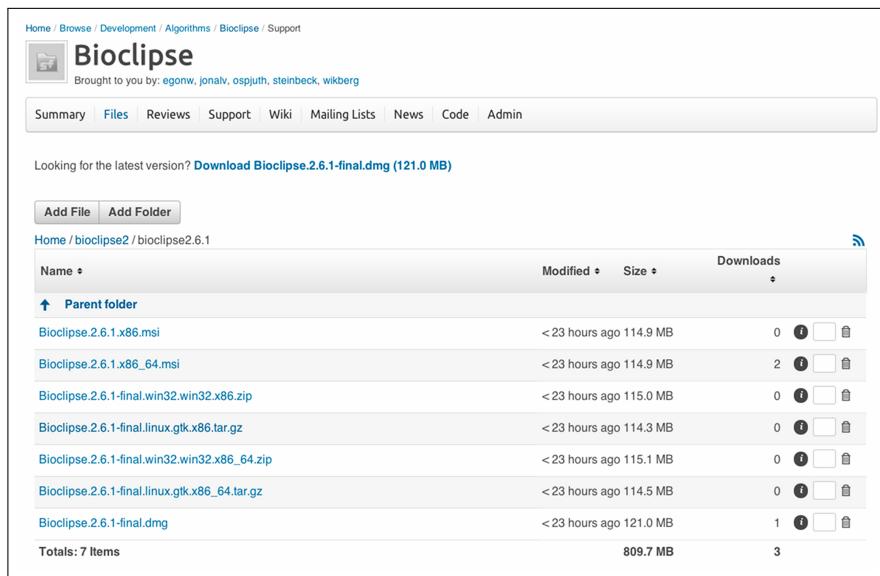
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Downloading

Bioclipse for Windows comes in a couple of different packages. Either as a .zip file or as an installation program and either as 32 or 64 bit. To find out if you have 32 or 64 bit in Windows xp and Windows 7 right click the icon named **My computer** and choose **properties**. On Windows 8 you need to go to **System and Security** and then **view basic information about your computer**. Normally, the installation program should be the obvious choice but if, for whatever reason, that doesn't work you can use the zip file. The Linux version is packaged as a tar.gz file and the Mac version comes as a .dmg file. These packages are available from:

<https://sourceforge.net/projects/bioclipse/files/bioclipse2/bioclipse2.6.1/>.



The screenshot shows the SourceForge project page for Bioclipse. At the top, there's a navigation bar with links to Home, Browse, Development, Algorithms, Bioclipse, and Support. Below the navigation is the Bioclipse logo and a message: "Brought to you by: egonw, jonalv, ospjuth, steinbeck, wikberg". A horizontal menu bar includes Summary, Files, Reviews, Support, Wiki, Mailing Lists, News, Code, and Admin. A sub-menu bar under "Files" shows "Home / bioclipse2 / bioclipse2.6.1". The main content area is titled "Looking for the latest version? Download Bioclipse.2.6.1-final.dmg (121.0 MB)". Below this, there are two buttons: "Add File" and "Add Folder". A table lists the available files:

Name	Modified	Size	Downloads
Bioclipse.2.6.1.x86.msi	< 23 hours ago	114.9 MB	0
Bioclipse.2.6.1.x86_64.msi	< 23 hours ago	114.9 MB	2
Bioclipse.2.6.1-final.win32.win32.x86.zip	< 23 hours ago	115.0 MB	0
Bioclipse.2.6.1-final.linux.gtk.x86.tar.gz	< 23 hours ago	114.3 MB	0
Bioclipse.2.6.1-final.win32.win32.x86_64.zip	< 23 hours ago	115.1 MB	0
Bioclipse.2.6.1-final.linux.gtk.x86_64.tar.gz	< 23 hours ago	114.5 MB	0
Bioclipse.2.6.1-final.dmg	< 23 hours ago	121.0 MB	1

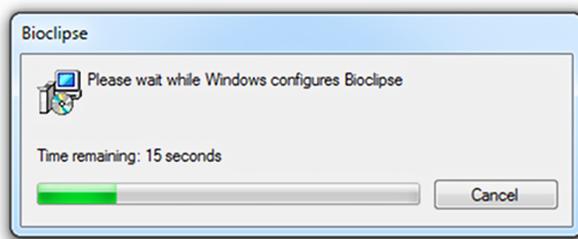
Total: 7 Items 809.7 MB 3 Downloads

Installing

The installation procedure differs between the operating systems. Bioclipse needs a Java installation to be present on the computer. To install Java, visit www.java.com and follow the instructions. If you are not sure whether or not you have Java, you can also check that on www.java.com.

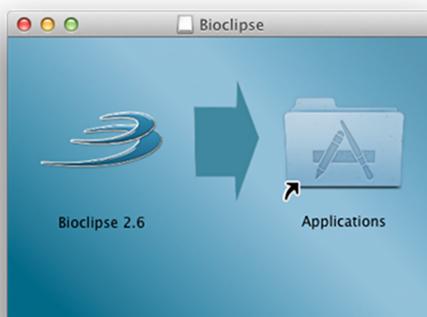
Windows XP, 7 and 8

If you downloaded Bioclipse as a .zip file you need to unzip it to a location where you want it and then start it from the Bioclipse.exe file. If you downloaded the installation program simply double click the file to start the installation program which will install Bioclipse on your machine and add it to the Start menu (on Windows xp, and Windows 7).



Mac OS X

The installation on Mac consists of dragging the .app file to the Applications folder. You then start Bioclipse from the Applications folder just like any other program.

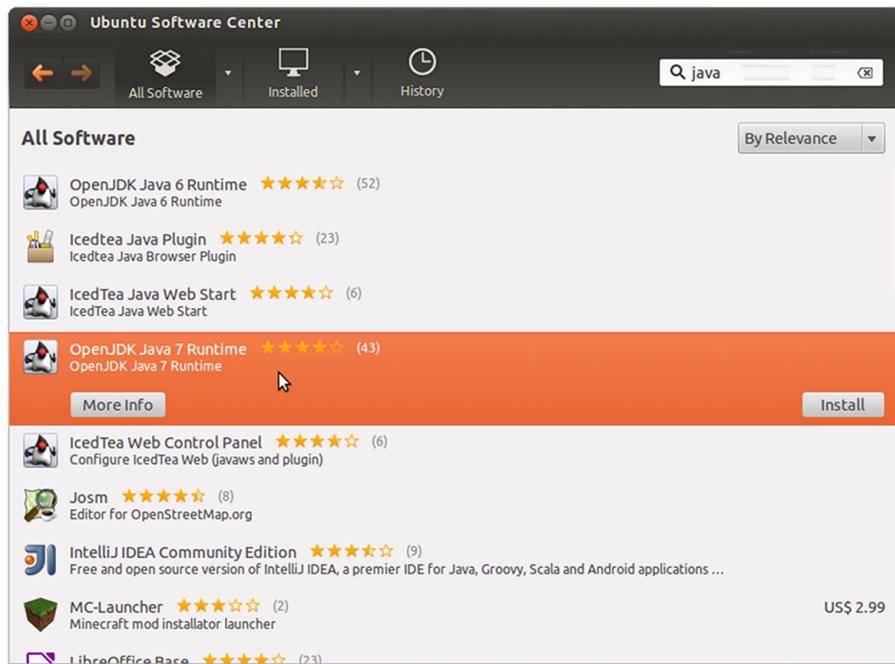


Ubuntu Linux

There is nothing special about the Linux distribution Ubuntu with regards to Bioclipse and it should work fine with other distributions as well. However we have tested Ubuntu and show how to get it running

on Ubuntu. Hopefully you can adapt the instructions to your local distribution. The Linux version of Bioclipse comes packed in a tar.gz file. All you need to do is to unpack the file to some suitable location and start from there. Bioclipse uses Java and has been tested with OpenJDK on Ubuntu Linux and Debian GNU/Linux.

OpenJDK can be found by searching for 'Java' at the Ubuntu software center. When you have found OpenJDK there, Java can be installed by just a simple click. The way to install OpenJDK can differ in other distributions of Linux, but as soon as you have installed OpenJDK Bioclipse should be runnable. When Java has been properly installed, Bioclipse can be started by double clicking the file named bioclipse.



Starting Bioclipse for the first time

When you start Bioclipse for the first time a Welcome page is shown.

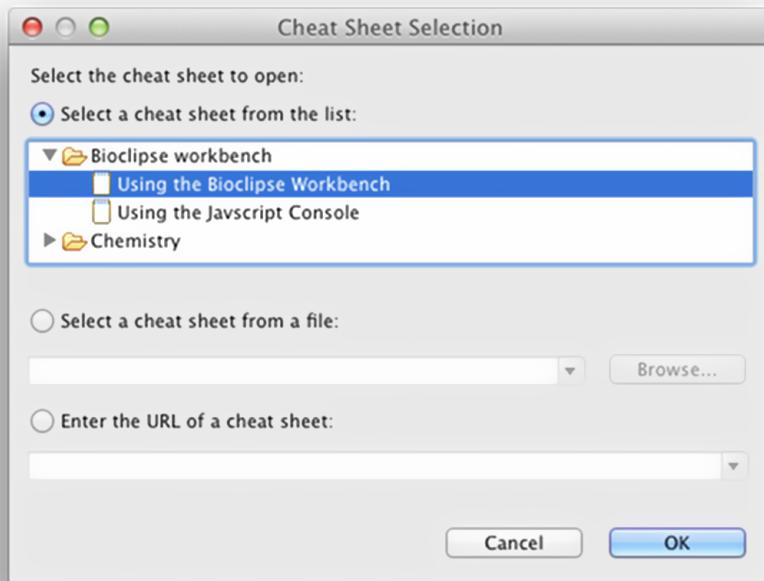


Spend some time looking at the various sub pages. Make sure to import the sample data if you want some data to play with. Just the empty workspace makes it difficult to test the different parts of Bioclipse.



The arrow in the upper corner brings you to the workbench. If you didn't try the [Introductory Bioclipse tutorial](#) from the Welcome page it is also reachable from the Help menu by choosing [Cheat Sheets](#) and then selecting the [Using the Bioclipse Workbench](#) cheat sheet. It might

be a good idea to spend some time following the instructions in this cheat sheet before you start exploring Bioclipse on your own.

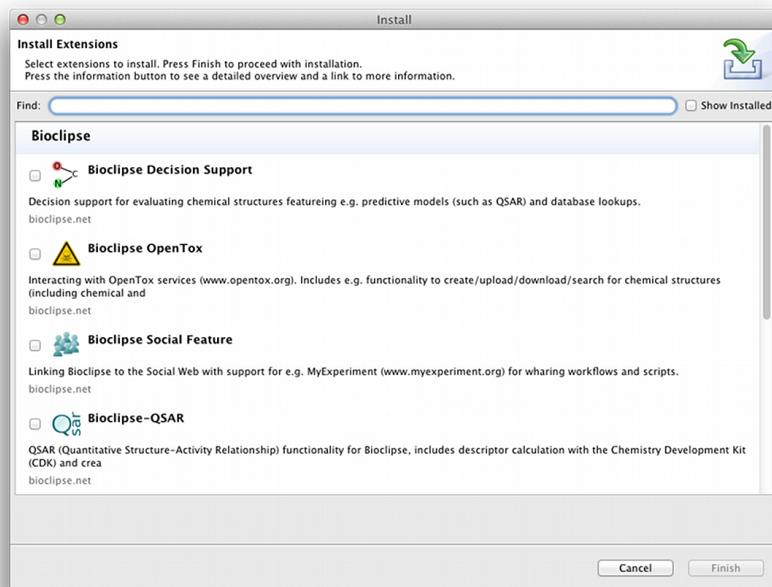


Updating and installing new features

Bioclipse is a highly customizable piece of software. New features and new versions of features can be installed as needed in your Bioclipse installation.

When Bioclipse starts, it checks the update site for new versions of what is already installed. If new versions are found, you are given the option to download them. If you choose to do so, the new versions will be downloaded. Once this is done, Bioclipse must be restarted to allow the new features to be used.

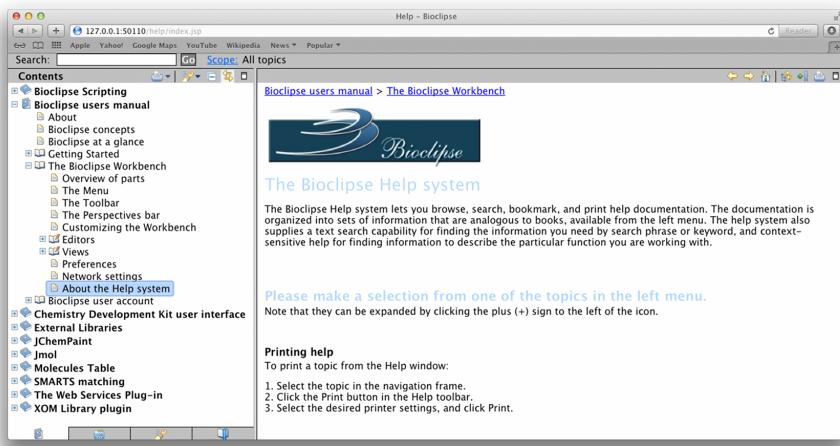
Bioclipse ships with, among other things, components for handling molecules but more advanced things like, for example, OpenTox support must be installed separately. To do this click [Install](#) in the top menu and then choose [New Feature...](#). This brings up a dialog showing all features available for installation. By clicking the check box named [Show installed](#) you can also see what features are already installed in your workbench.



Select what you want to install, accept the licenses and wait while Bioclipse restarts with the new features.

Getting help

There are multiple help features in Bioclipse. The main ones include the help pages in **HTML** and the cheat sheets. The Bioclipse Workbench cheat sheet was already mentioned earlier in this document but there are other ones explaining other things. When you install new features, new cheat sheets will be installed with them. To access the **HTML** help pages select **Help Contents** in the **Help** top menu.



You can browse the help pages from the list on the left and at the top left you can enter a search term of interest.

If there is something you can't find in the cheat sheets or the Help pages try sending a mail to: bioclipse-users@lists.sourceforge.net with your question.

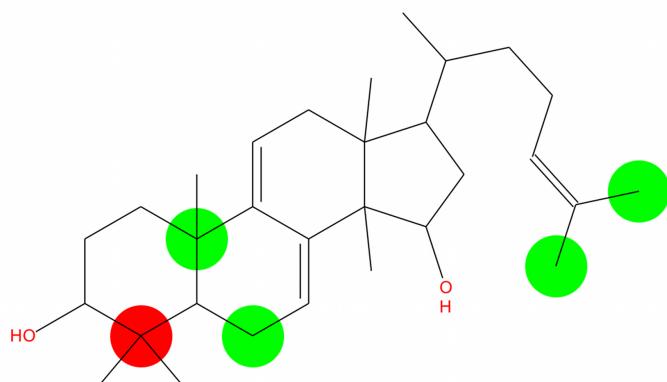
Installable Bioclipse features

Here follows a short explanation of what a few of the Bioclipse features available for installation can do.



MetaPrint2D

MetaPrint 2D is a tool to predict metabolic sites in chemical structures based on a large training set of CYP-mediated biotransformations.



L. Carlsson, O. Spjuth, S. Adams, R. Glenn, S. Boyer

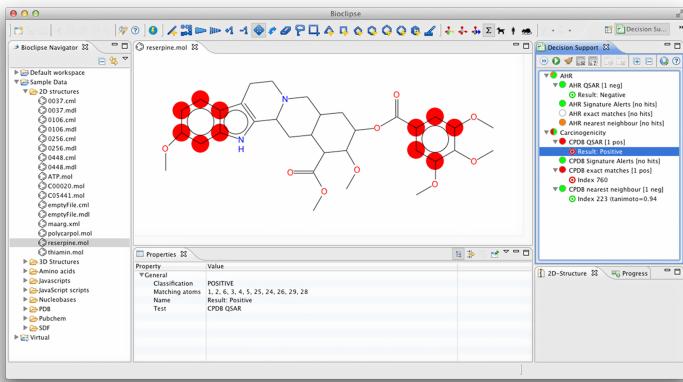
Use of Historic Metabolic Biotransformation Data as a Means of Anticipating Metabolic Sites Using MetaPrint2D and Bioclipse.

BMC Bioinformatics 2010, 11:362 [doi:10.1186/1471-2105-11-36](https://doi.org/10.1186/1471-2105-11-36).



Bioclipse Decision support

Bioclipse Decision support is a tool that provides a simple means to download and invoke predictive models on chemical structures. Model implementations include QSAR, Structural Alerts, exact and near neighbor matches, and proteochemometric models. Endpoints include Ames mutagenicity, Ahr, CYP 450, CPDB, daphnia, and hERG.



O. Spjuth, M. Eklund, E. Ahlberg Helgee, S. Boyer, and L. Carlsson
Integrated decision support for assessing chemical liabilities.

J. Chem. Inf. Model. 2011, 51 (8), pp 1840-1847 doi: [10.1021/ci200242c](https://doi.org/10.1021/ci200242c).



Bioclipse QSAR

Bioclipse QSAR comprises features for descriptor calculation and QSAR dataset creation in cdv and QSAR-ML formats. Descriptors are primarily CDK descriptors.

The screenshot shows the 'qsar.xml' project in the Bioclipse Navigator. The main window displays the 'QSAR responses' section with tabs for 'Information', 'Descriptors', 'Last build', and 'Responses'. Under 'Information', it shows 'Dataset name: N/A' and 'Authors: N/A'. Under 'Descriptors', it shows 'Descriptors: 4'. Under 'Last build', it shows 'Status: FINISHED', 'Calculation time: 0 s', and 'Autobuild is: OFF'. Under 'Responses', it shows 'Responses: 5' and 'Missing responses: 5'. At the bottom, there is a 'JavaScript Console' and a progress bar indicating 'No operations to display at this time.'

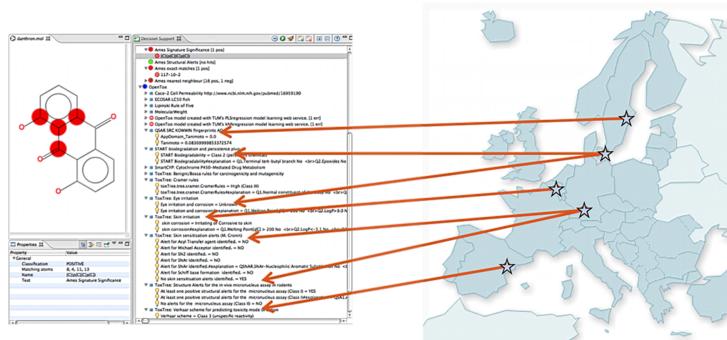
O. Spjuth, E. Willighagen, R. Guha, M. Eklund, J. Wikberg
Towards interoperable and reproducible QSAR analyses: Exchange of data sets

Journal of Cheminformatics 2010, 2:5, doi: [10.1021/ci200242c](https://doi.org/10.1021/ci200242c).



OpenTox

Bioclipse OpenTox provides tools to interact with the OpenTox infrastructure for predictive toxicology. Features include uploading/downloading chemical structures to OpenTox, and also the use of remote OpenTox predictive models in Bioclipse Decision Support.



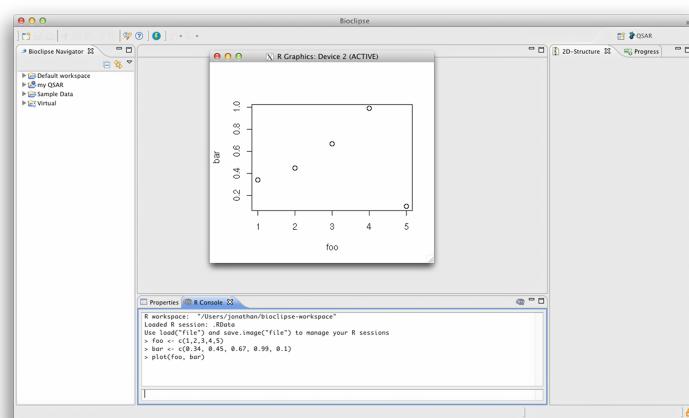
E. Willighagen N. Jeliazkova, B. Hardy, R. Grafström, and O. Sjöström.
Computational toxicology using the OpenTox application programming interface and Bioclipse.

BMC Research Notes 2011, 4:487 doi: 10.1186/1756-0500-4-487.



Bioclipse R

Bioclipse R integrates the statistical programming language R in Bioclipse.



O. Spjuth, V. Georgiev, L. Carlsson, J. Alvarsson, A. Berg, E. Willighagen, J.E.S. Wikberg and M. Eklund.

Bioclipse-R: Integrating management and visualization of life science data with statistical analysis.

Bioinformatics 2012, 29 (2), pages: 286-289. [doi:10.1093/bioinformatics/bts681..](https://doi.org/10.1093/bioinformatics/bts681)

Finally

If you use Bioclipse in your published scientific work please cite:

O. Spjuth, T. Helmus, E. Willighagen, S. Kuhn, M. Eklund, J. Wagener, P. Murray-Rust, C. Steinbeck, and J.E.S. Wikberg.

Bioclipse: an open source workbench for chemo- and bioinformatics.

BMC Bioinformatics, 2007, 8:59, [doi:10.1186/1471-2105-8-59](https://doi.org/10.1186/1471-2105-8-59).

O. Spjuth, J. Alvarsson, A. Berg, M. Eklund, S. Kuhn, C. Mäsk, G. Torrance, J. Wagener, E.L. Willighagen, C. Steinbeck, and J.E.S. Wikberg.

Bioclipse 2: A scriptable integration platform for the life sciences.

BMC Bioinformatics, 2009, 5:397, [doi:10.1186/1471-2105-10-397](https://doi.org/10.1186/1471-2105-10-397).

Web resources

<http://www.bioclipse.net/> Bioclipse web page.

<http://bioclipse.blogspot.se/> The Bioclipse blog.

<http://planet.bioclipse.net> Bioclipse planet -- syndication of Bioclipse related blogs.



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