

11 July 2013

BioBlender 1.0

Welcome to the new BioBlender. This new version is released as an add-on to the current version of Blender for Windows 7 or Linux Ubuntu 12 or newer.

In order to have all its functions working properly, BioBlender will need a few other software packages installed:

[Blender](#) 2.67 or newer

[ProDy](#)

[PyMOL](#)

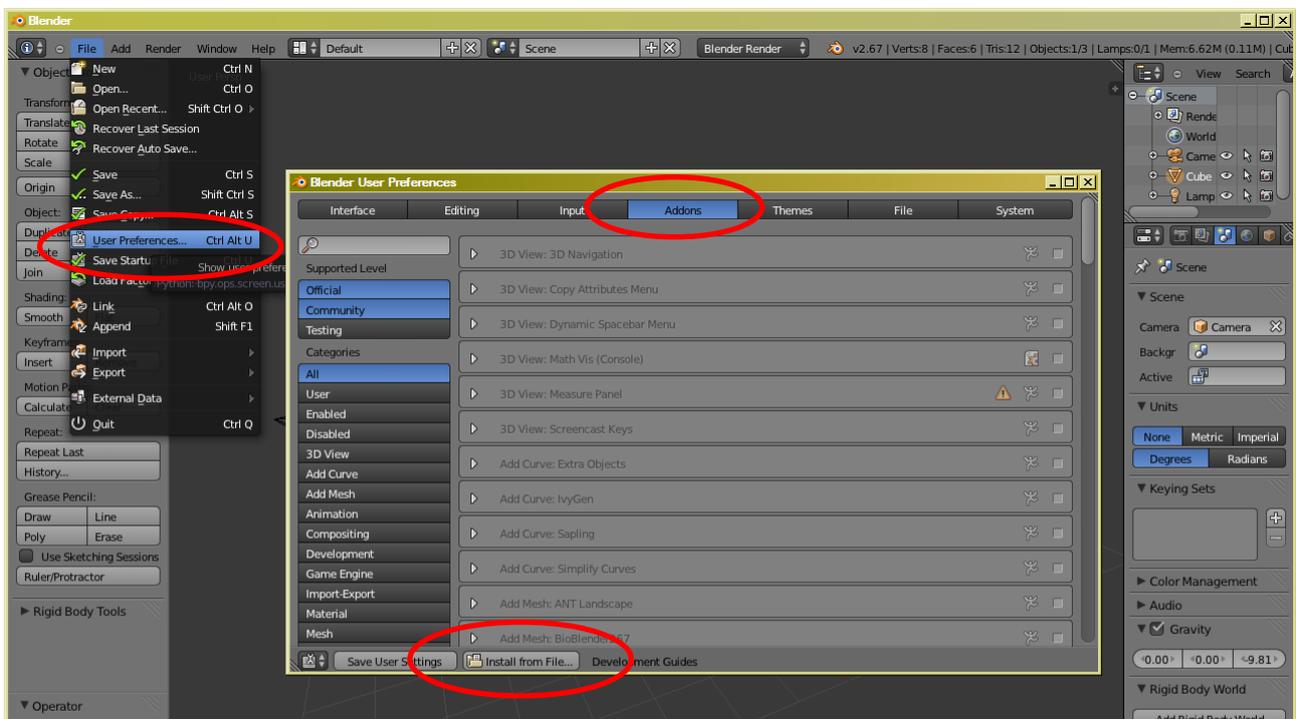
[Python](#) 2.6 or 2.7

NOTE for Windows Users: please see last page.

How to use BioBlender:

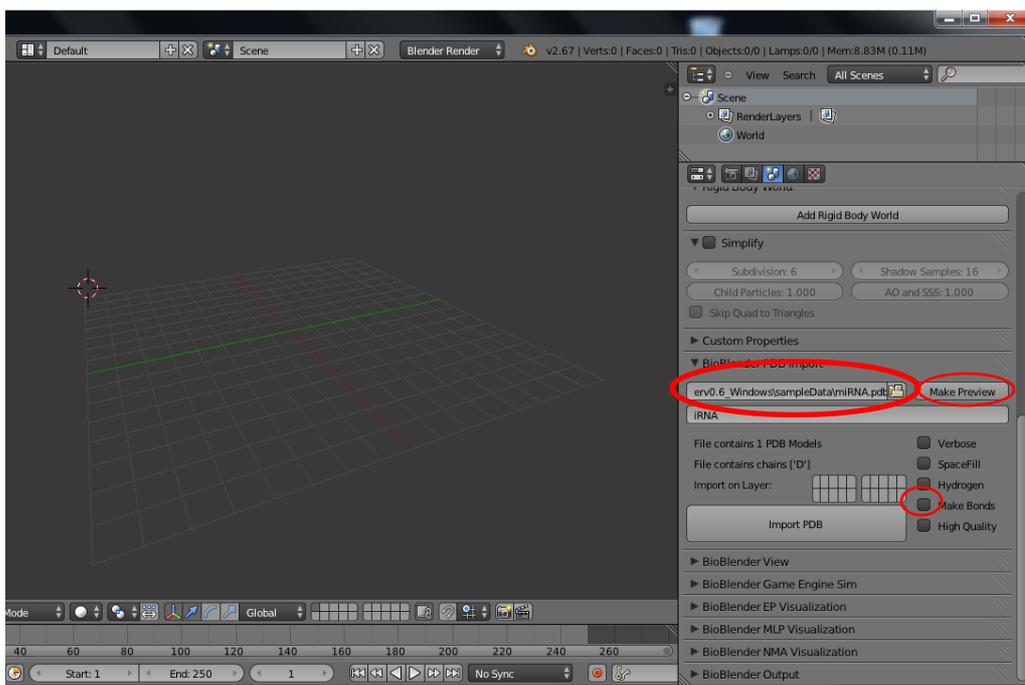
- Install Blender 2.67 or newer
- Download BioBlender 1.0, zipped (do not extract)

Open Blender and go to the **User Preference** panel (Ctrl+Alt+U), select tab **Addons**, click **Install from file**.



Locate the zipped BioBlender1.0.zip file, and activate it.

In the Scene panel, the BioBlender functions are now accessible.



(Eliminate from the default scene all object -Cube, Camera and Light- by pressing **a**, **x**, and **Enter**. You may want to save this starting scene, by pressing **Ctrl+u**).

Select a PDB file, either usign the 4 letter code (for PDB.org fetch), or browse in your own files. Click **Make Preview**, so that BioBlender can access the file, and provide relevant options:

- if your file is an NMR collection, BB will prompt you to select which models to import (up to 100), in which order, and how separate (how many frames between each model).

You may wish to activate the **Make Bonds**, to enable the creation of rigid body joints as chemical bonds, for more accurate animation when using the Game Engine (see below).

- if your file contains only one model (e.g. X-ray), with 1 or more chains, BioBlender will import all chains.

- if you wish to use the NMA feature (calculated by ProDy, wich must be installed in the computer independently), select the NMA parameters now. In case of NMR, ProDy will calculate NMA for the first Model in the NMR file.

Now everything is set to **Import PDB**.

This may take few seconds to a minute or so, depending on the size and complexity of your molecule. Together with the molecule, BioBlender add to the scene a set of lights and a camera. Press 0 to get a view form the camera, and adjust according to your need.

In the 3D viewport, your molecule can be built as atoms or surface. On the surface can be displayed the MLP and/or the EP.

To calculate these features use the BB panels MLP and EP, respectively. Here you can select the formula used for the calculi, the grid spacing (the finer the slower, but more accurate), and the particle density (for EP).

For animation, expand the **BioBlender Game Engne Sim** panel.

Set Collision to 1 to animate the molecule using the Game Engine,
Set Collision to 2 to also record the animation. Th motion will be recorded starting at frame F+200,
with F= the frame of the last uploaded conformation. I.e, if you imported 5 confomrations at 70
frames between each other, the last one is at frame 280, and the recording will start at frame 480.

The recorded conformations can be used for exporting the intermediate as pdb file or as a movie
(collection of PNG images). These options are set in the panel **BioBlender Output**, where you can
also select the frequency of export (export step) and the folder.

Please feel free to send us any comment on this program, by using the Blog in BioBlender website,
or mail us directly.

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Windows users:

please set the Python PATH in Environment Variables;
to do that, locate the python.exe file on your system (usually it is somewhere like C:\Python26\);
then open: Start - Control Panel - System and Maintenance - System - Advanced - Environment Variables - Variables;
choose "Path", click on "Modify" and append the python.exe path to the "Path" variable (e.g:
;C:\Python26\) (don't forget the semicolon at the beginning to separate the new path from others),
as shown in pictures below:

