How to set up your 3DM package.

This guide is for registered 3DM users that have a 3DM account. If you don’t have an account yet please first request a 3DM account here:

https://accounts.bio-prodict.nl/

The main steps to install your 3DM package are:

1. Request Yasara if you don’t already have Yasara. Otherwise update Yasara to the newest version.
2. Connect yasara with 3DM
3. Install Utopia

1a. Yasara installation instructions for new users:

If you are new to Yasara, go to www.yasara.org, select “Downloads” -> “Yasara for new users” and have a look which Yasara version you would like. The free “Yasara view” works only on the “Nuclear Receptors – ligand binding domain (Demo 2008)” 3DM system. All other versions work on all your 3DM databases. If you like to tryout Yasara with the 3DM module you can first request the free Yasara View and use it with the Nuclear Receptor database.

To get 3DM integrated with Yasara you have to type “3DM” in the “your middle initials” field (see figure 1). This is really important, do NOT forget this!!!!

Note: If you already downloaded YASARA once, don’t do it again, but request an update instead.
Figure 1. Example of a Yasara request by John Doe. Note the use of “3DM” at the middle initials field that is needed to include the 3DM plugin in the Yasara package.

After requesting Yasara you will get an email with download and installation instructions.

1b. Yasara installation instructions for existing Yasara users:

If you already are a Yasara user, please request an update via www.yasara.org to get the latest version. Make sure to type “3DM” in the “Update from Yasara version” field to have 3DM included in the Yasara package (see fig 2.). Correct examples are:
1.1.1 3DM
3DM 13.1.15
3DM

Figure 1. Example of a Yasara update request by John Doe. Note the use of “3DM” at the “Update from Yasara version” field that is needed to include the 3DM plugin in the Yasara package.

2. The Yasara 3DM connection:

After installing Yasara, you should have a 3DM option between the “Analyze” and “View” options (Figure 3). If not you possible have not installed the correct python version. You can update/get python directly from the help menu in Yasara (see figure 2). Use this to install python and restart Yasara. If you still don’t have the 3DM option, please let us know (support@bio-prodct.nl).
Figure 3. Yasara interface after installation of the 3DM plugin. Here the Help option was selected where Yasara offers the option the install python.

If you have requested the free Yasara View the 3DM-Yasara connection only works for the nuclear receptor ligand binding domain structures. You can try out how it works using nuclear receptor structures. For convenience we have prepared an example scene file containing two nuclear receptor structures which can be downloaded here: [https://3dm.bio-prodict.nl/guest-user/demo.sce](https://3dm.bio-prodict.nl/guest-user/demo.sce) and opened with Yasara (File -> Load -> Yasara Scene). Just try out the different 3DM options and see what happens. If asked for a password, use your 3DM credentials. You can also find 3DM data by right clicking on amino acids. Note that the data in the Heads Up Display is clickable to retrieve the underlying data (figure 4).

By selection structures from the 3DM system yasara will understand the 3D alignment numbering used in the 3DM alignment. This ensures the coupling of the structures to other data in the 3DM database. There are two ways to select structures from 3DM:

1. Use the 3DM option in Yasara -> “select data from 3DM” and give a PDB name (e.g. 1A28).
2. You can also select structures directly from the 3DM websites (first login via 3DM.bio-prodict.nl and select the nuclear receptors – ligand binding domain demo 2008 system or to your own 3DM if you have one). Once logged in you can export structures to Yasara by generating a Yasara scene file via the “visualize data in structure” ( ) option in the green banner once you have logged into the demo nuclear receptor 3DM system. This is how the example scene file was generated.
**Figure 3.** Yasara screenshot. Here mutations that are reported in literature to effect specificity are shown in red. Note that the heads up display on the top right contains links to the corresponding articles.
3. Installing Utopia Documents:

- Download Utopia from getutopia.com (Mac or Windows releases available: for Linux there is a beta-version which will probably work as well)
- Install the software

First, make sure Utopia has the right credentials:

- Run Utopia Documents
- Go to Edit - Preferences and click on the Plugins tab
- Put your 3DM username and password in the required fields
- Hit apply and close the preferences window
- Restart Utopia

Now open a paper.

- Download the demo paper from https://3dm.bio-prodict.nl/guest-user/demopaper.pdf and open it with Utopia.
- After a couple of seconds, a number of ‘boxes’ should appear on the right.
  Additional data about the paper is displayed here.
- Click on the ‘Bio-Prodict 3DM’ box, and select the “Nuclear receptor – Ligand binding domain (Demo 2008)” 3DM system to annotate this paper with (if you don’t see the Bio-Prodict box at this point you probably gave the wrong password)
- During the annotation you will see a white spinner in the blue bar on the left. When it is done the annotation process is complete. The first time you annotate a paper it can take up to 10 seconds, but after that it becomes quicker. If not, let us know.
- Scroll through the paper and hit the spacebar once in a while.
- The elements that are colored red are clickable. You can click on proteins, mutations and residues. You will see information retrieved from the 3DM database appears in the right banner. These things are again clickable. Just try them out and see how it works (see figure 3).
5. Prepare yourself!

After installing everything, please watch the demo movie and consult our publications at [www.bio-prodict.nl](http://www.bio-prodict.nl).

Please note that we regularly organize 3DM courses. 3DM is a complex program that has many powerful options. To get maximum value out of 3DM we advise to follow the 3DM/Yasara/Utopia course. These courses contain a large practical component in which participants solve real life problems from different fields (protein engineering, homology modeling, and drug design) with 3DM themselves. Information about the course can be found here: [http://www.bio-prodict.nl/#course](http://www.bio-prodict.nl/#course)


Enjoy 3DM!

The Bio-Prodict team!