

Quick Installation Guide of the ADOPS Virtual Disk

Go to <https://www.virtualbox.org/wiki/Downloads>, download the Oracle VirtualBox software version 4.1.20, and install it (by double clicking the VirtualBox icon). Go again to <https://www.virtualbox.org/wiki/Downloads>, download, and install the VirtualBox 4.1.20 Oracle VM VirtualBox Extension Pack.

Go to <http://sing.ei.uvigo.es/ADOPS/> and download the Ubuntu 12.04 (32 bits) Virtual Machine (~1GB) with a copy of ADOPS, T-Coffee, MrBayes and PAML already installed and configured. Extract the file to the folder of your choice.

Open VirtualBox and click on the **New** button and then on the **Next** button. Give a name to your virtual disk and under “Operating system” choose Linux (the Ubuntu version will be automatically selected). Click on the **Next** button.

Choose the amount of RAM memory to be allocated to the virtual disk. Do not be too greedy, otherwise the host system may crash. Do not choose too little RAM memory, otherwise it may take for ever to run ADOPS. About half of the available RAM memory is more than enough for most cases. Click on the **Next** button.

Choose the **Use existing disk** option and select the location of the file you extracted (by clicking on the icon that looks like a folder). Click on the **Open**, **Next**, and then **Create buttons**.

Click on the **Start** button. You are now running Ubuntu as a guest user. Your password is adops. ADOPS is installed under **Home**, but a shortcut is available on the desktop. Click on top of the shortcut. Start a new session by selecting the **Project** tab.

The Ubuntu virtual disk you just installed is fully functional, including the internet connection, and thus you can download the data from your preferred databases using the Ubuntu virtual disk. Nevertheless, it is possible to get access to the files on the host computer from this virtual disk. If you are using an USB pen, insert the device **after** starting the Ubuntu virtual disk only. Then go to devices (look at the top frame) and select USB devices. Click on top of the name of your USB pen. Your USB pen will be accessible (it may take up to 20 seconds to capture the USB port) under **Places**.

Remarks: Most of the content shown by ADOPS can be copied to a text file using the Ctrl + C option for copying and the Ctrl + V option for pasting. Figures can be exported in several formats. Everything is saved until you choose to delete the project and any project can be accessed using the **Load project** option. This way you can always look at the details of your analyses at any time.

At this time, ADOPS should be used with DNA sequences that do not have ambiguity codes only. In version 12.04, if present, ambiguity codes are replaced by an alignment

gap, that under some circumstances may lead to an erroneous alignment. We will tackle this issue in future ADOPS versions.

Please note that two of the alignment modes being made available (EXPRESSO and ACCURATE) require an internet connection. Depending on how your firewall is set up, they may not work properly.

If you use ADOPS, please read and cite the following article:

David Reboiro-Jato, Miguel Reboiro-Jato, Florentino Fdez-Riverola, Cristina P. Vieira, Nuno A. Fonseca and Jorge Vieira. ADOPS - Automatic Detection Of Positively Selected Sites. *Journal of Integrative Bioinformatics*, 9(3):200, 2012. Online Journal: http://journal.imbio.de/index.php?paper_id=200

Important remarks: ADOPS does not eliminate the limitations of the implemented software (T-Coffee, MrBayes and PAML). Avoiding very long project and experiment names and the use of short paths is likely a good option. CodeML will not run if stop codons are present in the sequence dataset, but the other software will run. Moreover, since this pipeline is intended for coding regions, sequences with a length that is not a multiple of three are not accepted. If you are running several CodeML models, and one of them does not converge, CodeML will unexpectedly exit, and ADOPS may exit as well.

Please send suggestions for improvements to Jorge Vieira (jbvieira@ibmc.up.pt) or to Miguel Reboiro-Jato (mrjato@uvigo.es).