

# Introduction: Getting started with VMD and controlling the display with button navigation windows

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This is just a brief summary, how to get started with using the program 'Visual Molecular Dynamics' (VMD) in connection with the script files in `vmdscripteng.zip` and `vmdscripteng.tar.gz`. (The contents of these two compressed files is identical!). To get a better insight what you are doing, please read the accompanying text: 'Improving presentations with the program 'Visual Molecular Dynamics' by controlling the display with the help of button navigation windows'.

## Installation:

- Make sure you have VMD properly installed on your system. If not, register, download and install it from <http://www.ks.uiuc.edu/Research/vmd/>.
- Unzip `vmdscripteng.zip`. A folder `vmdscripteng` should appear at the unzip location.
- If you are using Linux/Unix, you are ready to go, provided you start VMD from your home directory, either by calling it from the command line, or to start it by clicking the resp. button on your desktop. If you are using Windows or Mac-OS, you have to set all paths to the `pdb`-files in each `vmd-script` file to your personal path. The quickest way to do this is to use an editor, that can replace a text string in all loaded files at once. For example the freeware editors `notetab(-light)`, `crimson editor` or the shareware editor `winedt` can do the job.

All and only path names start with '`vmdscripteng/`', which you can replace by the appropriate location on your computer, for example by `C:/users/myname/vmdscripteng/`. Use forward-slashes! The rest of the path (`/pdbfiles/1abc.pdb`) should remain the same!

- Start VMD, goto File -> Load State and load one of the `*.vmd` -scripts. A protein should appear in the graphics display, and a button control window should be seen. Under Linux/Unix, you can also start one of the shell scripts `vmddemoeng.sh` bzw. `vmdteacheng.sh`. You can copy these scripts to your desktop and start from there. The shell scripts open a button control window with a selection of available VMD examples. These script files can be edited according to your demands.

If you can not see the protein, you likely made a mistake during the previous step. If you see the molecule, but the appearance and spining is awfully slow, check your graphics card and the drivers for OpenGL!

## Content of the scripts in vmdexample.zip

The following content list gives you a basic idea which biomolecule is depicted, and which pdb -files are used. A more thorough explanation of the examples is found in vmdinstruct.pdf.

The filename starts with a keyword, that may already give you a basic idea, which system is dealt with. After this keyword, the word button, radiobutton, hypertext or animation follows indicating the kind of presentation. In a button presentation, just a single keyword is shown in the button, characterizing the presentation initiated by pressing the resp. button. In hypertext and radiobutton presentation, whole sentences with explanations are given. If none of these words are given, the presentation is not button controlled, but merely is a standard vmd-script.

**antibodybutton.vmd:** 1fdl.pdb, 1igj.pdb, 1igt.pdb, 1ndg.pdb, 1yqv.pdb

Whole antibody, Digoxin binding FAB fragment as an example for small ligand binding, three different Anti -lysozyme FAB fragments with lysozyme bound, as an example for binding to a large antigen and to show the different binding geometries for the three monoclonal antibodies.

**aptamerbutton.vmd:** 1hao.pdb

Binding of 15mer DNA-aptamer to Thrombin, alternative binding site for a 29mer, quenching of TRP and TYR fluorescence by the two aptamers.

**atpsynthaseanimation.vmd:** 1c17.pdb, 1e79.pdb, 112p.pdb, 2a7u.pdb

ATP-synthase, animation showing the specific rotation of ATP-synthase

**bacterialrc.vmd:** 1pcr.pdb

Bacterial photosynthetic reaction center with cytochrome attached.

**bacteriorhodopsinanimation.vmd:** 1iw6.pdb, 1ixf.pdb, 1iw9.pdb, 1ucq.pdb

The cis -trans isomerization upon excitation as overlapping structures and as animation.

**bovinerhodopsin.vmd:** 1gzm.pdb

Mammalian vision pigment, no button control (yet)

**Designerproteinbutton.vmd:** 1qys.pdb

$\alpha$ -helix- $\beta$ -sheet structure artificially designed protein.

**DielsAlderRibozymebutton.vmd:** 1ykq.pdb, 1ykv.pdb, 1y1s.pdb

Artificially designed, catalytically active RNA with and without substrate

**ElongFactortrnabutton.vmd:** 1ttt.pdb

Protein - t-RNA complex, tertiary structure of RNA, modified nucleobases.

**gfpbutton.vmd:** 1emb.pdb

wt-Green Fluorescent Protein, proton network relevant for the understanding of the photophysical properties and for ESPT

**gfpswitchanimation.vmd:** 1a53.pdb, 1a56.pdb

GFP analogue protein asFP595, photoswitching shown as overlap of cis-trans isomerization and animation.

**hollidayjunction.vmd:** 1crx.pdb, 2crx.pdb, 3crx.pdb, 4crx.pdb, 1p4e.pdb

Holliday junction constructs, starting, intermediate and final state

**phototropinanimation.vmd:** 1n9l.pdb, 1n9o.pdb

Phototropin light detection mechanism, reversible forming of covalent bond between the flavin chromophore and a cysteine sulfur atom in its neighborhood.

**psIIbutton.vmd, psIIradiobutton.vmd, psIIhypertext.vmd:** 1s5l.pdb

PhotosystemII -complex, mit all antennapigments and the Mn-Cluster The RC -Komplex D<sub>1</sub>D<sub>2</sub> is enhanced.

**pypanimation.vmd:** 1s1y.pdb, 1s1z.pdb, 1otb.pdb

Photoactive Yellow Protein (PYP) photoswitching displayed as overlap of cis-trans isomerization and animation.

**rclh1button.vmd:** 1pyh.pdb, 1kzu.pdb

Reaction center antenna complex, containing LHI/RC and separatly, presentation of LHII

**ribosomebutton.vmd:** 1jgp.pdb, 1giy.pdb

Overall ribosome structure containing the protein and r-RNA backbone, and three t-RNA in atomic resolution translating a piece of m-RNA.

**ricedwarfvirus.vmd:** 1uf2.pdb

Complete viral structure, no buttons (yet)