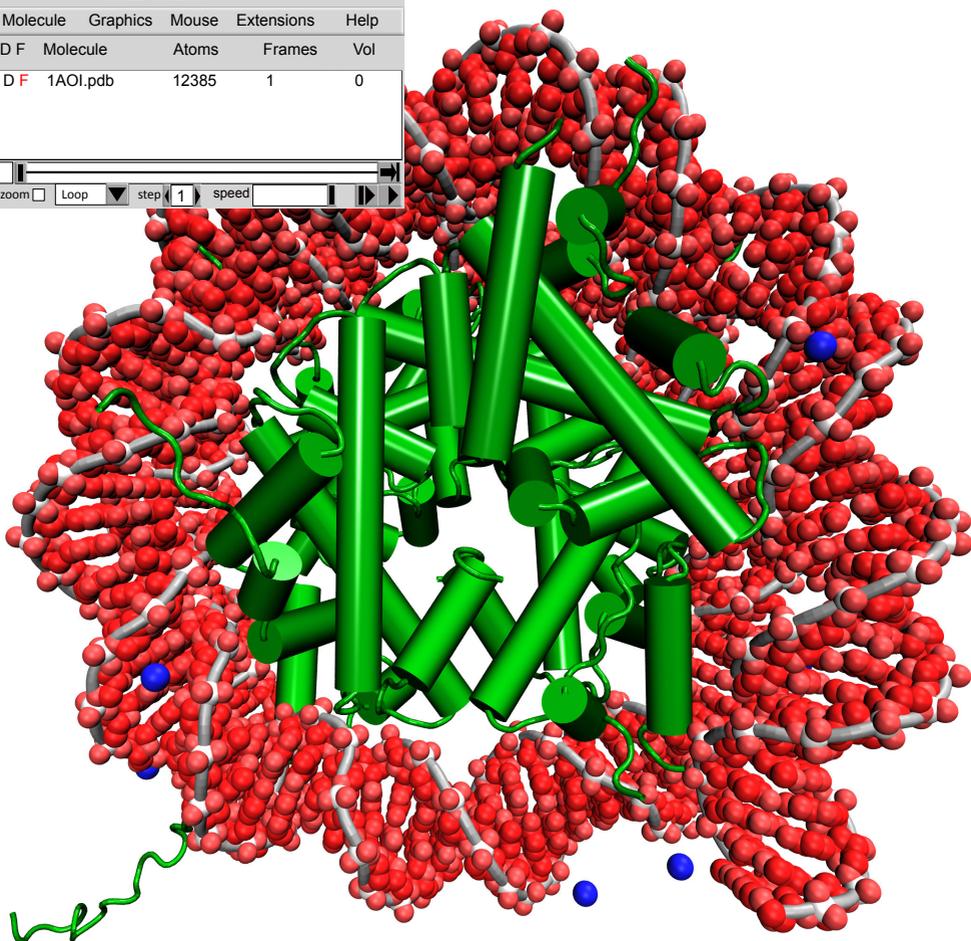


## VMD Main

File Molecule Graphics Mouse Extensions Help

ID T A D F Molecule Atoms Frames Vol

16 T A D F 1AOI.pdb 12385 1 0

zoom  Loop step 1 speed**VMD**

tools for

**Computational Chemistry**



# PREFACE

In this leaflet are presented a new set of computational tools for biomolecular simulations. All the software applications were developed to find new and innovative ways to deploy new technologies for computational chemistry and biochemistry with an unyielding commitment to continually improve our current understanding about science.

All of these tools have been included in the popular VMD software as plugins or as stand alone applications and can be freely downloaded using the VMDStore software available at:

*[github.com/portobiocomp/vmdStore](https://github.com/portobiocomp/vmdStore)*

Nuno M. F. S. A. Cerqueira ([nscerque@fc.up.pt](mailto:nscerque@fc.up.pt))

Sérgio F. Sousa ([sergio.sousa@fc.up.pt](mailto:sergio.sousa@fc.up.pt))

André F. Pina ([apina@fc.up.pt](mailto:apina@fc.up.pt))

Carla S. S. Teixeira ([carla.teixeira@fc.up.pt](mailto:carla.teixeira@fc.up.pt))

Henrique S. Fernandes ([henrique.fernandes@fc.up.pt](mailto:henrique.fernandes@fc.up.pt))

Juliana F. Rocha ([juliana.rocha@fc.up.pt](mailto:juliana.rocha@fc.up.pt))

**2018**





# VMD Store

## DESCRIPTION

vmdStore provides a centralised repository for all the VMD plugins with a dedicated user-friendly interface that runs directly on VMD. This allows the VMD users to install all the software application that are developed for VMD and keep them updated on their machines. It also provides a new framework to turn the development of new VMD plug-ins easier, avoid multiple copies of these codes, minimize security risks and enable easy backup.

## SCREENSHOTS

Developed by Henrique S. Fernandes and Nuno M. F. S. A. Cerqueira - PortobiComp

**CITATION**

*to be published*

**DOWNLOAD**

[github.com/portobiocomp/vmdStore](https://github.com/portobiocomp/vmdStore)



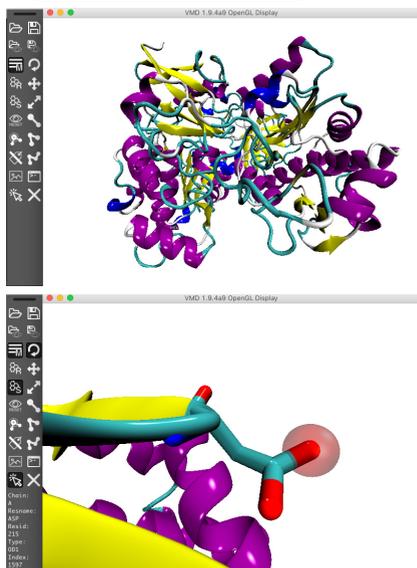


# toolBar

## DESCRIPTION

VMD is an exceptional program to visualise molecular structures. The main drawback of this software is the learning curve required to master the system of keywords and commands. The toolBar was developed to turn VMD more user-friendly and a more productive tool. In addition, a new set of functionalities were added, namely a new selection manager, which includes a new selection engine with syntax highlight and auto-completion, a new rendering GUI that enhances the creation of state-of-the-art image on VMD, etc.

## SCREENSHOTS



Molecule ID: 0: 2nap  
Selection Tree:  
none  
chain A  
protein  
4: ARG  
5: PRO  
6: GLU  
7: LYS  
8: TRP  
9: VAL  
10: LYS  
11: GLY  
12: VAL  
13: CYS  
14: ARG  
15: TYR  
16: CYS  
17: GLY  
18: THR

Atom Selection:  
(chain A and ((protein and ((resid 9))))  
Add Apply

#	Atom Selections
0	X  all
1	X  resid 215

Draw Style  
Drawing Method: Licorice  
Coloring Method: Name  
Help Options

Molecule ID: 0: 2nap  
Selection Tree:  
none  
chain A  
resid 215

Atom Selection:  
resid 215  
Add Apply

#	Atom Selections
0	X  all
1	X  resid 215

Show/Hide  
Zoom  
Number of Atoms  
Delete

Draw Style  
Drawing Method: Licorice  
Coloring Method: Name  
Help Options

**CITATION**

*to be published*

**DOWNLOAD**

[github.com/portobiocomp/toolBar](https://github.com/portobiocomp/toolBar)



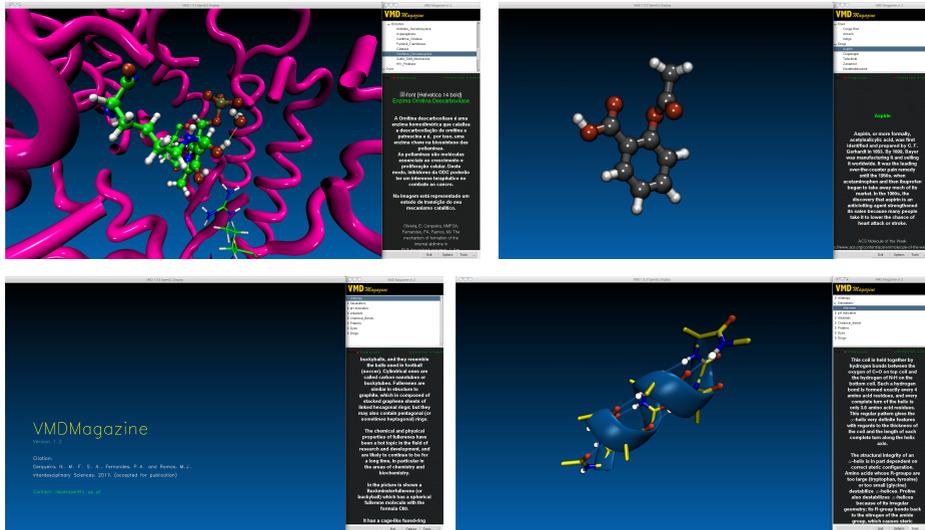


# VMD Magazine

## DESCRIPTION

Visualization can be a motivating way of teaching students about the microscopic world. This can become even more exciting if the information is based on accurate computational results rather than on crude approximations that eventually might create unreal alternative perceptions. vmdMagazine was developed to turn computational simulations into stunning high-impact video presentations, suitable for classes/lectures and even conferences.

## SCREENSHOTS



## CITATION

*Interdisciplinary Sciences: Computational Life Sciences* (2017), 1-6.  
DOI: 10.1007/s12539-017-0255-2

## DOWNLOAD

[github.com/portobiocomp/vmdMagazine](https://github.com/portobiocomp/vmdMagazine)





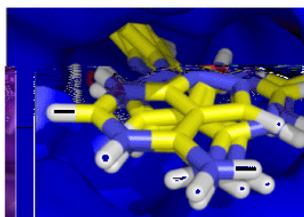
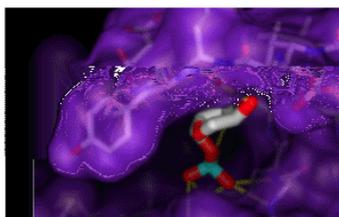
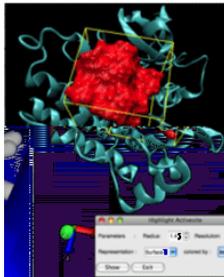
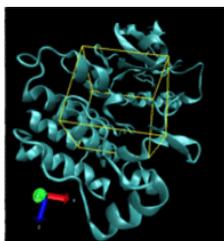
# VSLAB

## DESCRIPTION

VSLAB (Virtual Screening LABORatory) is a graphical interface for the well known molecular docking software AutoGrid/AutoDock that has been included into VMD as a plug-in. This program allows the user to prepare and analyse the results from simple molecular docking runs or more complex virtual screening campaigns.

The potential associated to this software makes it an attractive choice not only for educational purposes, but also for more advanced users that can use VSLAB to increase workflow and productivity on everyday tasks.

## SCREENSHOTS



## CITATION

*Int. J. Quantum Chem.* (2011), 111: 1208–1212.  
DOI: 10.1002/qua.22738

## DOWNLOAD

[github.com/portobiocomp/vsLab](https://github.com/portobiocomp/vsLab)



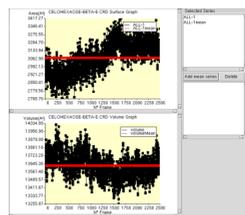
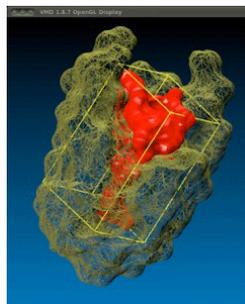
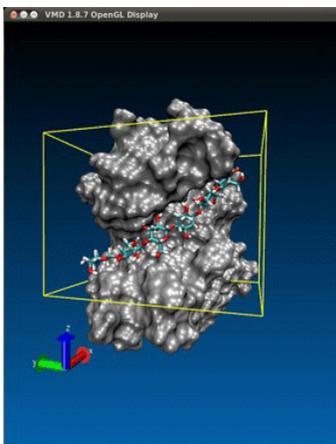
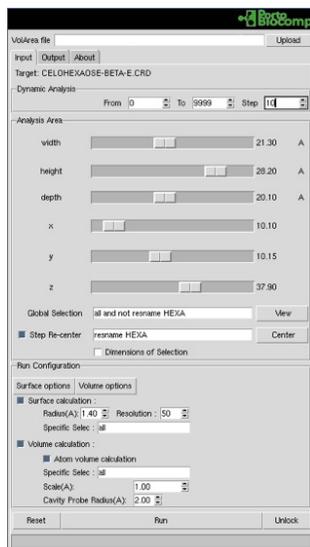


# VolArea

## DESCRIPTION

VolArea is a VMD plug-in that calculates the volume as well as the surface area of any chemical structure. The volume can be used to predict the space occupied by any chemical structure as well as that of cavities, such as tunnels, clefts, etc. The surface area can be used to map or calculate the exposed area of a chemical structure to the solvent or to another chemical structure. This is particularly useful to characterize protein:ligand complexes or corresponding binding sites, as well as protein:protein interfaces.

## SCREENSHOTS



## CITATION

*Chem Biol Drug Des* (2013), 82: 743–755.  
DOI: 10.1111/cbdd.12197

## DOWNLOAD

[github.com/portobiocomp/volArea](https://github.com/portobiocomp/volArea)



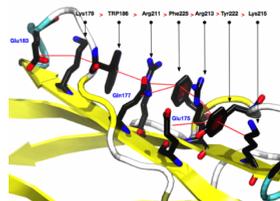
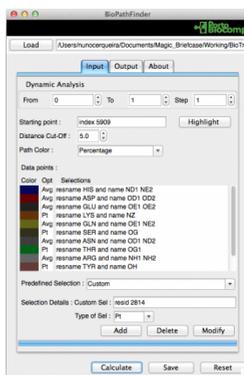
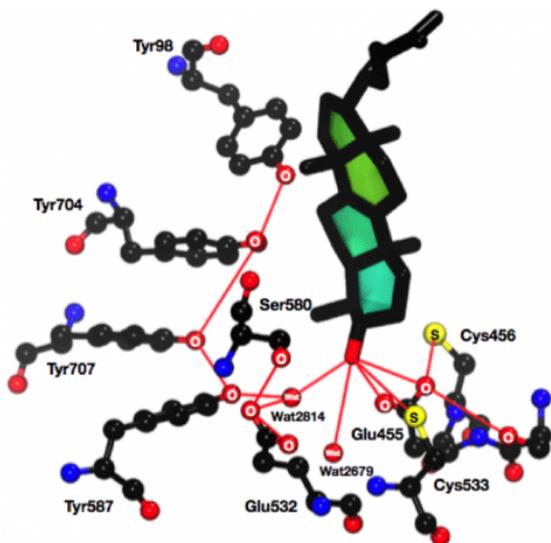


# Chem-Path-Tracker

## DESCRIPTION

Chem-Path-Tracker is a bioinformatic tool that was developed to locate functionally relevant chemical motifs in protein structures. The chemical motifs can be a small group of residues or structured protein fragments with highly conserved properties that have important biological functions. The analysis is based on atoms/residues pair distances applying a modified version of Dijkstra's algorithm that can be applied to static structure or in molecular dynamics simulations.

## SCREENSHOTS



## CITATION

*Chem Biol Drug Des* (2014), 84: 44–53.  
DOI: 10.1111/cbdd.12349

## DOWNLOAD

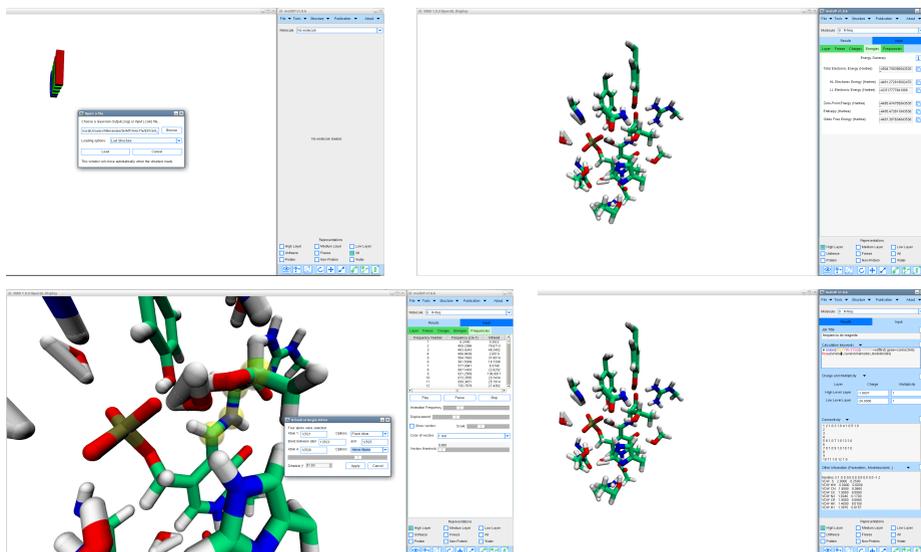
[github.com/portobiocomp/chemPathTracker](https://github.com/portobiocomp/chemPathTracker)



## DESCRIPTION

molUP is a VMD plugin that offers a complete set of tools that enhance the preparation of QM and ONIOM (QM/MM, QM/QM, and QM/QM/MM) calculations. The starting structures for these calculations can be imported from different chemical formats. A set of tools is available to help the user to examine or modify any geometry parameter. This includes the definition of layers in ONIOM calculations, choosing fixed atoms during geometry optimizations, the recalculation or adjustment of atomic charges, performing SCANS or IRC calculations, etc. molUP also extracts the geometries from the output files as well as the energies of each of them. All of these tasks are performed in an interactive GUI that is extremely helpful for the user.

## SCREENSHOTS



## CITATION

*Journal of Computational Chemistry* (2018)  
DOI: 10.1002/jcc.25189

## DOWNLOAD

[github.com/portobiocomp/molUP](https://github.com/portobiocomp/molUP)





[www.biosim.pt](http://www.biosim.pt)