

VMD Store—A VMD Plugin to Browse, Discover, and Install VMD Extensions

Henrique S. Fernandes,¹ Sérgio F. Sousa,¹ and Nuno M. F. S. A. Cerqueira*

UCIBIO@REQUIMTE, BioSIM, Departamento de Biomedicina, Faculdade de Medicina da Universidade do Porto, Alameda Professor Hernâni Monteiro, 4200-319 Porto, Portugal

Supporting Information

ABSTRACT: Herein we present the VMD Store, an open-source VMD plugin that simplifies the way that users browse, discover, install, update, and uninstall extensions for the Visual Molecular Dynamics (VMD) software. The VMD Store obtains data about all the indexed VMD extensions hosted on GitHub and presents a one-click mechanism to install and configure VMD extensions. This plugin arises in an attempt to aggregate all VMD extensions into a single platform. The VMD Store is available, free of charge, for Windows, macOS, and Linux at <https://biosim.pt/software/> and requires VMD 1.9.3 (or later).



1. INTRODUCTION

Computing has revolutionized the way that we do research, and the role played by computer simulations no longer can be underestimated in science. Today, there is a myriad of computational tools that allow scientists to answer a wide range of scientific problems. The use of these computational tools has become routine for several tasks such as molecular simulations, molecular docking, hybrid quantum mechanical/molecular mechanics (QM/MM) studies, etc.

The availability of more powerful hardware allows computer simulations to produce more and better data. Moreover, data can also be subjected to a more detailed analysis.

Most of these developments would not be possible without the advances in molecular computer visualization. Those advances allowed computational (bio)chemists today to analyze very complex data and present the results in a readily understandable form, generating new knowledge that can be successfully used to design new experiments, develop new materials, and validate previous results.

In the past 20 years, this evolution has been partially helped by the development of several specialized software applications such as Visual Molecular Dynamics (VMD),¹ UCSF Chimera,² PyMol,³ Coot,⁴ and CCP4 mg.⁵ All these programs enable a detailed visualization of the molecular systems. VMD is one of the most popular computational software programs, counting more than 16 000 citations since 1994 (according to the Thomson Reuters Web of Science database). VMD's popularity is a consequence of its powerful capabilities and free distribution. Notwithstanding, VMD allows an easy interaction with the Tcl scripting language, enabling the development of additional extensions, programmed in the Tcl/Tk language. This means that users can develop their own scripts/extensions working with VMD,

according to their needs. This possibility gave rise to a flourishing community of VMD plugin developers and users, all around the world.

Over the last ten years, several VMD extensions have been developed and published. Notable examples include WAT-CLUST,⁶ Epock,⁷ molUP,⁸ PyContact (standalone software that interacts with VMD),⁹ vsLab,¹⁰ RIP-MD,¹¹ ChemPath-Tracker,¹² METAGUI 3,¹³ vmdMagazine,¹⁴ CaFE,¹⁵ VolArea,¹⁶ TopoGromacs,¹⁷ vmdICE,¹⁹ SIRAH tools,²⁰ and DelPhi Force,²¹ among others.¹⁸ However, all these plugins are spread over the Internet on several different websites. The lack of a general repository and the poor indexing of those websites by the search engines contributes to make their discovery difficult. In many cases, the files become lost, either because the authors no longer support them, have changed university or research group, or the website was shut down. Another important point is the update of the plugins, which is often challenging to follow, and it is imperative to maintain the availability and compatibility of the plugins. Moreover, the installation procedure is usually distinct among different plugins, and the VMD Store ensures that the user does not need to be concerned about that since the process is automated.

VMD already provides a complete set of tools built into the standard distribution. However, many more have been developed as plugins and are not included in the standard distribution. All of these plugins provide new features that greatly enhance the capabilities of VMD, involving a large community of individual plugin developers and users, scattered around the world, in the creation of new possibilities of application of VMD, including new solutions, new methods,

Received: September 3, 2019

Published: October 21, 2019

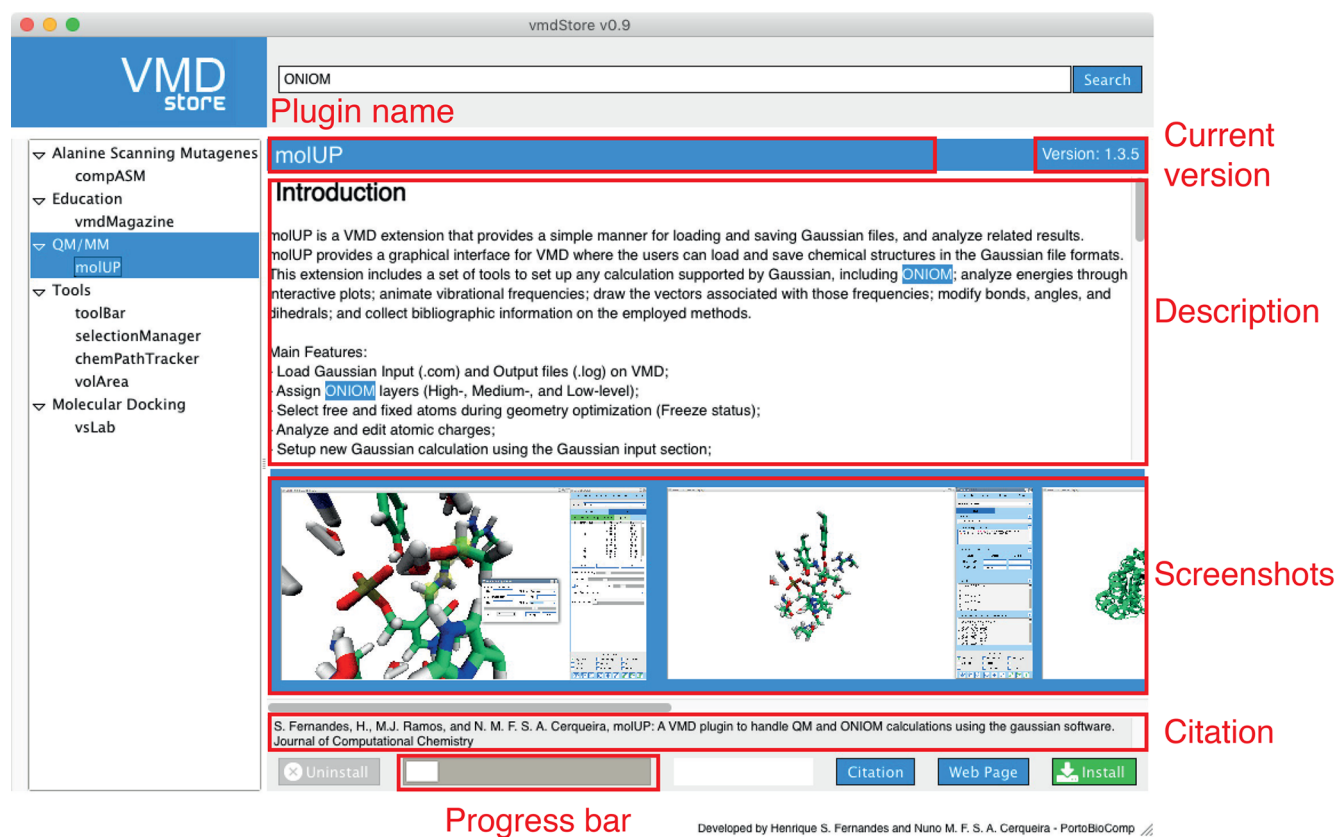


Figure 1. Main window of a plugin on the VMD Store. On the left panel, a list of all available plugins is presented organized by category. In the main section, the VMD Store provides information about the plugin's name, latest version, description, screenshots, and citation. Moreover, there are buttons to install or uninstall the plugin, as well as, links for the citable paper and its repository on GitHub.

new chemical problems, or more user-friendly ways to perform specific tasks. These new capabilities strength VMD's native capabilities and improve its ability to handle other tasks such as the preparation and analysis of calculations with quantum mechanics, ONIOM QM/MM, protein–ligand and protein–protein docking, virtual screening, molecular mechanics, and molecular dynamics, as well as structural analysis, with different external software packages.

Most of these plugins were published in several scientific journals, which means that they have already been fully and extensively validated scientifically. Some of these plugins are very useful for beginner or advanced scientists, but many times, they are not available due to the reasons that were described above.

Hereupon, we decided to develop the VMD Store, an independent open-source VMD plugin that allows VMD users to browse, discover, install, and manage other VMD plugins, connecting the individual plugin developers with the VMD plugin users.

2. VMD STORE

The VMD Store is a free and open-source extension for VMD that allows the searching, installation, updating, and uninstallation of VMD extensions in an easy (one-click) fashion. The VMD Store works locally on the user machine but requires an Internet connection to collect all the data to install or update the plugin.

The VMD Store is an independent open-source plugin developed by us as part of the community of VMD users and for the community of VMD users.

2.1. Install the VMD Store. The first step to use the VMD Store is to install it. A step-by-step tutorial is available at <https://biosim.pt/how-to-install-vmd-store/> that explains how to install the VMD Store manually from the source code in any operating system. On the website, <https://biosim.pt/software/>, the binary versions of the installer are also available. This allows any user to install the VMD Store on Windows, macOS, and Linux operating systems.

After the successful installation of the VMD Store, the users can access it through the “Extensions” > “VMD Store” > “VMD Store” menu of VMD.

2.2. VMD Store GUI. The startup window of the VMD Store is composed of a header where the logo and a search bar are placed.

Below the header, the VMD Store GUI has a left sidebar containing the list of VMD extensions available on the VMD store. VMD plugins are classified in different categories facilitating the search of specific applications by the user. On the right side is the main section where the information about a certain plugin is loaded. As soon as the user selects one plugin from the “List of VMD extensions”, the VMD Store promptly gets, from the online repository, all the information about that plugin. This information includes the plugin name and the currently available version. Afterward, a description of the plugin is provided, as well as some screenshots of the

plugin. The users can click on the screenshots and see them in a magnified picture gallery.

The footer section includes some relevant information about the plugin such as the citation (if available), the link to the article (“Citation” button), and the link to the developer’s web page (“Web Page” button). Moreover, there are also two important buttons, the “Install” and “Uninstall” buttons, that allow users to install or remove the selected plugin, respectively (Figure 1).

The search bar allows the users to quickly search for any term on the VMD Store database and check if any available plugin matches the provided keywords. The plugins that match the search pattern are highlighted (blue background) on the “List of VMD extensions” section of the GUI. When one of the plugins is selected, a full description of the VMD extension is provided, as well as, a button that allows its installation through a single click (Figure 1).

2.3. VMD Store System—GitHub Based. The VMD Store works based on the code repository GitHub (<https://github.com/>), which is one of the biggest software development platforms in the world. This platform is particularly interesting because it is used worldwide, and it is also free.

Therefore, the VMD Store, which is also hosted on GitHub, collects all the data from GitHub repositories. The VMD Store will index all repositories that are listed on the “Available Plugins” section of the VMD Store repository. Each repository is associated solely to one plugin that is shown in the “List of VMD extensions” of the VMD Store GUI (Figure 1). Once the user selects a certain plugin, the VMD Store collects all the available data from the respective repository on GitHub, such as the plugin name, the latest version available, the description (from the “README.md” file), and the screenshots (from the “Screenshots” directory). When the “Install” button is pressed, the installation procedure is started, and it downloads the *Latest release* package (not the “master branch”) available on that GitHub repository. The files are automatically unpacked and placed on the user’s machine, and the content of the “install.txt” file is placed on an internal file of the VMD Store. This file is called every time the VMD starts, loading the installed plugins. The “install.txt” file contains all commands required to load the VMD plugin, and it can be edited by plugin developers to load additional libraries. Those libraries can be other Tcl packages or compiled binaries such as *.dll* or *.exe*.

So far, the VMD Store looks at repositories of VMD plugins developed in our research group, the DelPhiForce²¹ plugin developed by Emil Alexov et al., and the Pathways²² plugin by Ilya Balabin et al. However, the VMD Store is prepared to include other VMD plugins developed by other groups in order to aggregate all possible VMD extensions in a single platform. Efforts are being conducted to invite more developers to include their plugins in the VMD Store database.

Since the VMD Store is lodged at GitHub, different developers can have their own code on their own repositories and yet the VMD Store can index them and install them from those “independent” locations. In this way, developers can keep their code updated with no barriers or delays since the VMD Store will automatically check all the indexed repositories.

In these cases, a few requirements must be followed by the developers in order to make their repositories compatible with the VMD Store, namely:

- Make the code available on a public GitHub repository.
- The repository must follow the structure described above to allow VMD Store indexing (Figure 2).

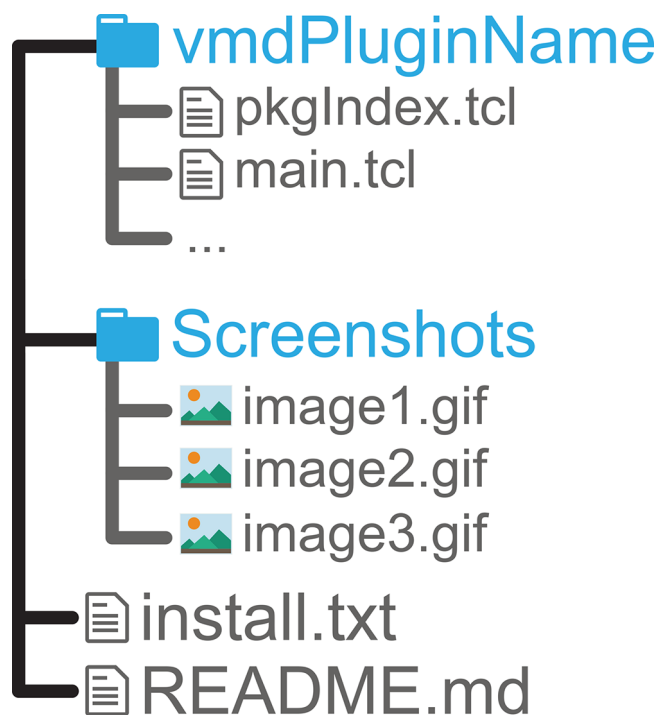


Figure 2. Directory and file organization required by the VMD Store to index a plugin. All the files related to the plugin must be placed inside a directory, named by the plugin’s name, in the root of the repository. Then, a set of screenshots (name scheme: *imageX.gif*) must be placed in a directory, named *Screenshots*, on the root of the repository. The root of the repository should also include two files: *install.txt*, containing all required commands to start the plugin, and *README.md*, containing the description and relevant information about the plugin.

- Contact the authors of the VMD store to include the new repository in the indexing process of the VMD Store.

One important feature of the VMD Store is to provide a singular manner to promote VMD plugins, ensuring that the credits are attributed to the authors of the plugin. This is done through the inclusion of the proper citation and the web page where the article describing the plugin is available.

A detailed guide, which explains how the GitHub repository must be organized, is provided in the [Supporting Information](#).

2.4. Installation of Plugins. Any VMD extension available on the VMD store can be installed simply clicking on the green “Install” button placed in the bottom of the VMD Store window. The VMD Store will automatically download and install the plugin. After a successful installation, a message will pop up informing that the user must restart VMD to make the new plugin available (Figure 3 A). The plugin becomes available through the VMD menu “Extensions” > “VMD Store” > “Plugin’s name”. After the installation, the “Uninstall” button becomes available allowing the user to remove the plugin, and the “Install” button is changed to a “Re-Install” that erases the local installation and repeats the installation process (Figure 3 B). When the developer releases a new update, the VMD Store

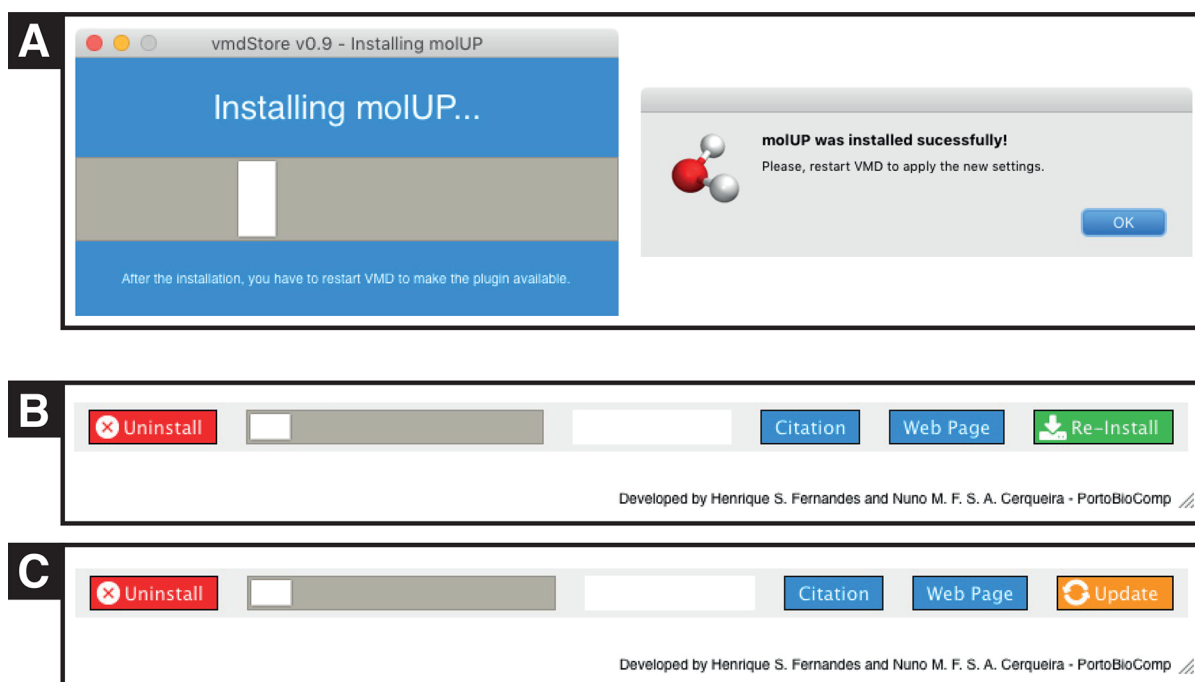


Figure 3. (A) Two sequential windows are displayed during the installation process of a plugin using the VMD Store. (B) Footer section after the installation of a certain plugin. The buttons available allow the uninstallation or reinstallation of the plugin, as well as, access to the citable publication and GitHub repository. (C) In case an update is available for a certain plugin, the “Re-Install” button is replaced by the “Update” button.

will show an orange “Update” button that alerts the user for this update (Figure 3 C).

In short, the process is simple as described above, letting the users install, uninstall, and update their VMD plugins by clicking on a single button.

3. TECHNICAL IMPLEMENTATION

The VMD Store was developed in Tcl/Tk, the native language used on VMD extensions, and all required libraries are provided to ensure that the user does not have to install any software/library other than the VMD. It requires the version 1.9.3 or above of the VMD. The VMD Store is directly integrated into the “Extensions” menu of the VMD from where it opens the GUI.

The VMD Store come with an installer software to make the installation process very easy.

The VMD Store is compatible with the following operating systems: Windows, macOS, and Linux.

The VMD Store requires an Internet connection to communicate with the online repositories.

4. CONCLUSION

VMD is one of the most used tools by (bio)chemists, in particular computational (bio)chemists, because it provides a set of powerful tools to analyze chemical and biological systems. Moreover, this software enables the integration of other scripts and plugins made by VMD users to improve its native capabilities. Although several plugins have been developed and published over the past few years, there is no way to access to all of them easily. This was the main motivation to develop the VMD Store. In this way, the VMD Store aims to improve the engagement between the VMD users and the developers of VMD plugins. Making the VMD plugins easily discovered, installed, and updated, the VMD

Store potentiates the continued expansion of the set of external VMD plugins. Consequently, more VMD plugins are available to complement VMD to face more (bio)chemical problems.

The community of VMD users can actively contribute to this set of plugins and make them available through the VMD Store.

■ ASSOCIATED CONTENT

● Supporting Information

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acs.jcim.9b00739.

Detailed scheme about the GitHub repositories' architecture (PDF)

■ AUTHOR INFORMATION

Corresponding Author

*Email: nunoscerqueira@med.up.pt.

ORCID

Henrique S. Fernandes: 0000-0002-9280-1838

Sérgio F. Sousa: 0000-0002-6560-5284

Notes

The authors declare no competing financial interest.

■ ACKNOWLEDGMENTS

European Union (FEDER funds POCI/01/0145/FEDER/007728) and National Funds (FCT/MEC, Fundação para a Ciência e Tecnologia and Ministério da Educação e Ciência) under the Partnership Agreement PT2020 UID/MULTI/04378/2013.UID/MULTI/04378/2013; NORTE-01-0145-FEDER-000024, supported by Norte Portugal Regional Operational Programme (NORTE 2020), under the PORTUGAL 2020 Partnership Agreement, through the European Regional Development Fund (ERDF); and Fundação para a

Ciência e a Tecnologia (FCT) through projects IF/01310/2013 are acknowledged. Henrique Fernandes is grateful to the Fundação para a Ciência e Tecnologia (FCT), Portugal, for a PhD Grant (SFRH/BD/115396/2016). We want to thank all the developers of VMD plugins that collaborated with us during the development of the VMD Store. Additionally, we would like to encourage all developers to add their external VMD plugins to the VMD Store.

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