

Article

molVisual3D: A standalone executable software for 3D visualization of molecules

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Abstract

In this article, a standalone executable software molVisual3D, for 3D visualization of molecules was developed. It uses the XYZ file of a molecule to generate its 3D graphics. Some parameters can be specified by the user. In the generated 3D graphics window, the user can right- or left-click mouse to zoom in or zoom out the 3D graphics, or mouse-drag the graphics to rotate the 3D graphics, or slide scrollbar to vertically or horizontally translate the 3D graphics. The 3D graphics can be saved into an image file (in BMP format). Both molVisual3D and demonstration data files were given.

Keywords 3D visualization; molecules; objects; standalone software; biology; chemistry.

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1 Introduction

So far, numerous visualization software, e.g., the software for network visualization, have been developed (Narad et al., 2017; Zhang, 2007, 2021, 2023, 2024a-g). Some of them were developed as Java tools, e.g., I developed a Java software for 3D visualization of objects and molecules, based on JDK 1.1 and J2SDK 1.4.2 (Zhang, 2023). Matlab software were also developed for free uses (Zhang, 2021). In the recent, some standalone executable software were developed by using Delphi (Zhang, 2024e-g). Java and Matlab are powerful for developing software tools and thus be widely used. Nevertheless, the JRE and Matlab environment are needed to support these Java and Matlab software respectively. Delphi, which is based on Object Pascal, is the development environment for standalone software. For example, I have developed the standalone executable software for 3D visualization of objects using Delphi (Zhang, 2024e). In present study, I developed a standalone executable software for visualization of molecules. It uses the XYZ file of a molecule to generate the 3D graphics. The full Delphi codes, the free software and demonstration data files were given.

2 Software and User Guide

2.1 Software codes

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