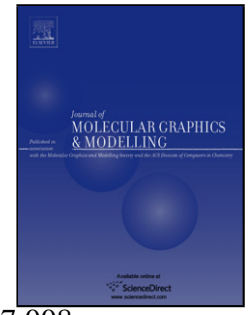

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Open Source Molecular Modeling

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Abstract

The success of molecular modeling and computational chemistry efforts are, by definition, dependent on quality software applications. Open source software development provides many advantages to users of modeling applications, not the least of which is that the software is free and completely extendable. In this review we categorize, enumerate, and describe available open source software packages for molecular modeling and computational chemistry.

1. Introduction

What is Open Source?

Free and open source software (FOSS) is software that is both considered "free software," as defined by the Free Software Foundation (`http://fsf.org`) and "open source," as defined by the Open Source Initiative (`http://opensource.org`). The distinctions between free and open source software are largely philosophical - the free software movement is primary motivated by user freedoms ("free as in speech, not free as in beer") while the open source movement is more concerned with promoting an open development model to enhance software quality. However, as a practical matter, especially with regards to scientific software, such distinctions remain philosophical rather than practical as the most popular software licenses are both free and open source.

The unifying theme of open source software licenses is that they allow users to use, modify, and distribute software without significant restrictions. This is achieved by making the full source code of the software available to users. Broadly speaking, open source licenses

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