Easy-to-use, offline Molecular Dynamic preparation graphical interface with VTX_2026

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VTX[1][2] is an open source molecular visualization software capable of handling most molecular structures and dynamics trajectories, regardless of their file formats or system size. It features a real-time high-performance molecular graphics engine, based on modern OpenGL and Cuda, optimized for the visualization of massive molecular systems and molecular dynamics trajectories. In the present work, we highlight a graphical user interface that supports Molecular Dynamic simulation (MD) setup, allowing non-expert users to parametrize a system in real time to run a MD. VTX currently supports system preparation for GROMACS[3] MD engine. Binaries for Windows and Ubuntu Linux are available at http://vtx.drugdesign.fr. VTX source code is available at https://github.com/VTX-Molecular-Visualization.

Bibliography :

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