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# iTube Studio

## 7.4.0.5

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#### **iTunes Studio 7.4.0.5**

The three-dimensional structure of TPS obtained from the predicted model using the Phyre2 server was energy-minimized using the Protein Preparation Wizard in the Schrödinger suite (version 2019-3: Schrödinger, New York, NY). The Schrödinger suite (version 2019-3) is a

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collection of integrated programs for molecular modeling, design, and analysis that are based on the OPLS-AA (Optimized Potentials for Liquid Simulations all Atom), developed by the force field group at the University of Illinois at Chicago [ 24, 25 ]. It comprises a set of non-commercial software packages, including Maestro, Schrödinger, Avogadro, and LigandScout, with protein preparation modules. The protein preparation wizard is a tool for preparing the protein structure for molecular dynamics simulations, molecular docking, and drug design. The preparation wizard guides the user through the initial steps of protein geometry optimization in an automated fashion to optimize the protein structure using the OPLS-AA force field (OPLS-AA force field for short). The simulation module of Discovery Studio 2019 is mainly used for the molecular dynamics

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of macromolecular systems (docking and molecular simulation). The simulation module of Discovery Studio 2019 is mainly used for the molecular dynamics of macromolecular systems (docking and molecular simulation). The molecular dynamics (MD) simulation was performed using the OpenMM package [ 30 ] with the molecular mechanics CHARMM force field [ 31 ] in the Standard Dynamics Cascade protocol in Discovery Studio 2019 (BIOVIA). The solvent box was constructed using the Solvent Builder module of Discovery Studio 2019. The system was gradually heated from 50 K to 278 K over 50 ps and equilibrated at this temperature. Further dynamics simulations (2 ns) were performed according to the OpenMM of dynamics (production) protocol. The coordinates of each atom were saved every 4 ps, thus producing a trajectory size of 500 snapshots. The trajectories were analyzed

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using the analysis trajectory protocol of Discovery Studio 2019. Structures were visualized and rendered using Discovery Studio 2019. 5ec8ef588b

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