

Schrödinger Suite 2012 Update 2 Documentation

Solutions and Workflows

- *Induced Fit Docking*
- *Ligand and Structure-Based Descriptors*
- *P450 Site of Metabolism*
- *QM-Polarized Ligand Docking*
- *Virtual Screening Workflow*

Quick Reference

- *Glide Docking*
- *Ligand Preparation*
- *LigPrep Command Options*
- *Job Options Supported, by Product*
- *Phase Command-Line Database Tasks*
- *Phase Command-Line Pharmacophore Modeling*
- *Phase Pharmacophore Modeling in Maestro*
- *Preparing a Library of Compounds for Glide or Phase*
- *Protein Preparation*
- *QikProp Descriptors and Properties*
- *Recommended Settings for Jaguar*
- *Running Distributed Schrödinger Jobs*
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- *Setting Up a License Server*

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- *Semiempirical NDDO Guide*
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- *BioLuminate User Manual*
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- *Canvas User Manual*
- *Canvas Python API*

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- *CombiGlide User Manual*
- *CombiGlide Quick Start Guide*

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- *ConfGen User Manual*

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- *Desmond User's Guide* (from D. E. Shaw Research)
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- *Jaguar User Manual*
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- *MacroModel User Manual*
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