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BioLuminate ®. Zhu, K.; Day, T.; Warshaviak, D.; Murrett, C.; Friesner, R.; Pearlman, D., "Antibody structure determination using a combination of homology modeling ...

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This manual contains exercises designed to help you learn the basic tasks you will need to prepare and initiate Jaguar calculations from Maestro. For more information about Jaguar features, see the Jaguar User Manual. This chapter contains instructions for setting up the tutorial.

Jaguar Quick Start Guide

The first such algorithm of its kind, QM-Polarized Ligand Docking uses ab initio methodology to calculate ligand charges within the protein environment. Innovative and practical, QM-Polarized Ligand Docking offers substantially enhanced accuracy over pure MM docking algorithms.

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