Data Management System for Distributed Virtual Screening

Supporting Information

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DOCKING DETAILS

Before docking, the atom-specific affinity map files were created by AutoGrid.[1] The numbers of points in the x, y, and z directions were 62, 52, and 42, respectively, and the spacing between two adjacent grid points was 0.25 Å. The AutoDock[2] program was used to produce poses for further minimization and the custom ranking (Zhou et al., in preparation). To speed up the calculation, the maximum number of energy evaluations was set to 25000. The docking was followed by CHARMM[3] minimization using the CHARMm force field.[4] To suggest enough poses for minimization and testing of the ranking protocol, the hybrid genetic algorithm in AutoDock was run 400 times with different initial seeds. The poses were minimized with the rigid protein after docking, and the duplicated poses were eliminated by clustering using an all-atom RMSD cutoff of 0.01 Å.

THE ESTIMATION OF THE MAXIMUM AMOUNT OF MOLECULES DISTRIBUTED PER SECONDS FOR THE MPI VERSION OF DOCK

The estimation is based on "High Throughput Computing Validation for Drug Discovery Using the DOCK Program on A Massively Parallel System"[5] where the authors used a subset of 27005 drug-like ligands as a benchmark. Supposing that the efficiency of the "master" of MPI-DOCK is 100%, which is the upper limit, it took about 50000 seconds to finish docking on 256 Blue Gene/L processors. By increasing the number of processors to 16384, the efficiency diminished to about 55% due to the

overload of the master. Therefore, the maximum amount of molecules distributed per seconds is about 19, which is calculated by $27005 \Big/ \left(\frac{50000 \times 256}{55\% \times 16384} \right)$.

REFERENCES

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