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System Construction and actual performance report of the virtual screening on grid computing system using Windows desktop machines.

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NTT DATA and Accelrys Japan launched the large scale virtual screening pilot project using 561 human proteins and 2,140 drugs which aims to validate *in silico* approach to the prediction of drug-protein interactions in association with RIKEN Genomic Sciences Center from Aug 1, 2003. This project also aims to access the performance of the recently developed docking method using "LigandFit" and the PC-grid computing system "cell computing". This paper shows typical system's related performance issue and their solution. Computation was carried out by a cluster setup composed of 400 desktops PCs provided by the company and the university. In 176 days, docking simulation for each combination of 561 already known human proteins structure and 2,140 drugs taken from MDDR database was carried out. The maximum performance of the grid system was 350 GFlops. In the system operation aspect, the job scheduling method was improved with visualization tool for computational status of client PC, in which system performance increased by 30%. This project shows that the PC grid computing approach and molecular docking method are suitable for large-scale computation of drug-protein interactions.