

## **Structure-based drug discovery on Grid**

GAP Virtual Screening Service (GVSS) is a large scale in-silico high throughput drug screening platform deployed on the gLite environment. In addition to supply intensive computing power, it enhanced effective data management and docking job monitoring. In the past two years, it conducted Avain Influenza drug refinement and Dengue Fever drug discovery on EUAsiaGrid. Exploring the virtual screening service and learning how to handle various proteins and ligands compound libraries were enhanced since these years. We study the complex protein – ligand interactions based on these experiences. We do the fundamental researches about protein – ligand interactions based on the PDDBind database. Our first target is to deal with proteins which molecular weight less than 300, then classifying the results by ligand characteristics. Then, one can evaluate the proper type of protein which is suitable to the GVSS scoring function. On the other hand, those unsuitable proteins will be judged by other scoring function. Molecular docking simulation is a time consuming process to search exhaustively all correct conformations of a compound. However, the massive in silico processes benefit from the high throughput computing grid technology. On the e-infrastructure (EUAsia VO), the docking work will be done ahead of time. Furthermore, these activities also facilitates more biomedical e-Science applications, such as other diseases and compounds profiling.

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