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High Throughput Interactive In-Silico Drug Discovery Platform: GVSS-2

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Description of the Work

The GVSS-2 has two new features: One is the automation of pre-requisite process and the other is the new protein structure database. In order to run the AutoDock virtual screening, the Biomedical scientists need to convert the ligan files from "mol2"to "pdbq"format before submitting the virtual screening job. Via GVSS-2, users only need to upload their "mol2"files, then the system would convert the "mol2"format into "pdbq" automatically. While extracting information in mol2 file, the system also pre-calculates ligand physicochemical descriptors such as Atom Count, Molecular Weight, Aromatic Ring Count, etc. With the pre-calculation descriptors, users would get the results back in clustered category. It is more efficient and easier for users to examine their results. Moreover, users could implement advanced ligand filter, such as similarityduring libaray preparation and retrieve the results based on the physicochemical descriptors. GVSS-2 features a new function for classifying protein structure via its PDBID annotated in the PDB bank. The new protein structure database has been added into the GVSS-2., In addition, we provide online tools for users to decide the docking site and to generate energy map files of various atom types.

Conclusions

To enable the large-scale highthroughput molecular docking running on an e-Science infrastructure, ASGC developed the GVSS application package. The newly released GVSS-2 is upgraded with new functions, including automation of pre-requisite process and addition of classified protein structure database. Users can select the proteins/ligands, visualize the docking sites and binding sites, generate the energy map files and retrieve docking results based on the physicochemical properties.

Impact

Different from the standalone GVSS, the GVSS-2 is incorporated with enhanced Graphical User Interface (GUI) application. Through the GUI, the end users can easily take advantage of Grid computing or Desktop Grid computing resources to conduct a large-scale virtual screening for drug. With the help of the high performance computing and huge data managing capabilities of the distributed computing resources, possible chemical components can be screened and studied very rapidly by the available computer modelling applications. This will help medicinal chemists to concentrate on the most promising chemical components, the ones they expect to have the greatest impact.

Overview (For the conference guide)

Molecular docking simulation is a time consuming process to search exhaustively all conformation of a compound. However, the massive in-silico process has benefitted from the high throughput computing technology.

To provide intensive computing power and effective management, we developed an in-silico drug discovery platform –GVSS (GAP Virtual Screening Service) by taking advantage of global e-Science infrastructure such as EUAsiaGrid and EGI. To improve the accessibility of the distributing computing resources, service grid and desktop grid , ASGC developed the GVSS-2 empowered by GAP-2 with the new functions of automation of pre-requisite process and adding new protein structure database.

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