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Development and application of a platform for drug discovery using grid technology and XML database

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A number of computer resources, such as CPUs and storages, can be connected over networks to construct a huge virtual computing environment using grid technologies. Our project “g-Drug Discovery” aims to develop a platform for drug discovery using grid technologies, on which various analysis and calculations are conducted, such as molecular mechanics method, replica exchange method, docking with proteins, molecular orbital method, and 3-dimensional quantitative structure activity relationship.

For this aim we have developed Xsi-G, a grid-based version of Xsi, which is a a suite for virtual screening based on Molecular Mechanics (MM). Xsi is a kind of software that integrates various methods for ligand based and structure based drug design, such as calculation of structure and energy of molecule, docking simulation, 2-dimensional and 3-dimensional structure descriptor calculation, and machine learning by the support vector machines. A useful computer aided drug design software requires the control of various type of information and fuctions. Xsi can flexibly control these information by “Xsi Script”, which is a simple objective script language. For the middleware for grid technology, we utilize a grid RPC system “OmniRPC”.