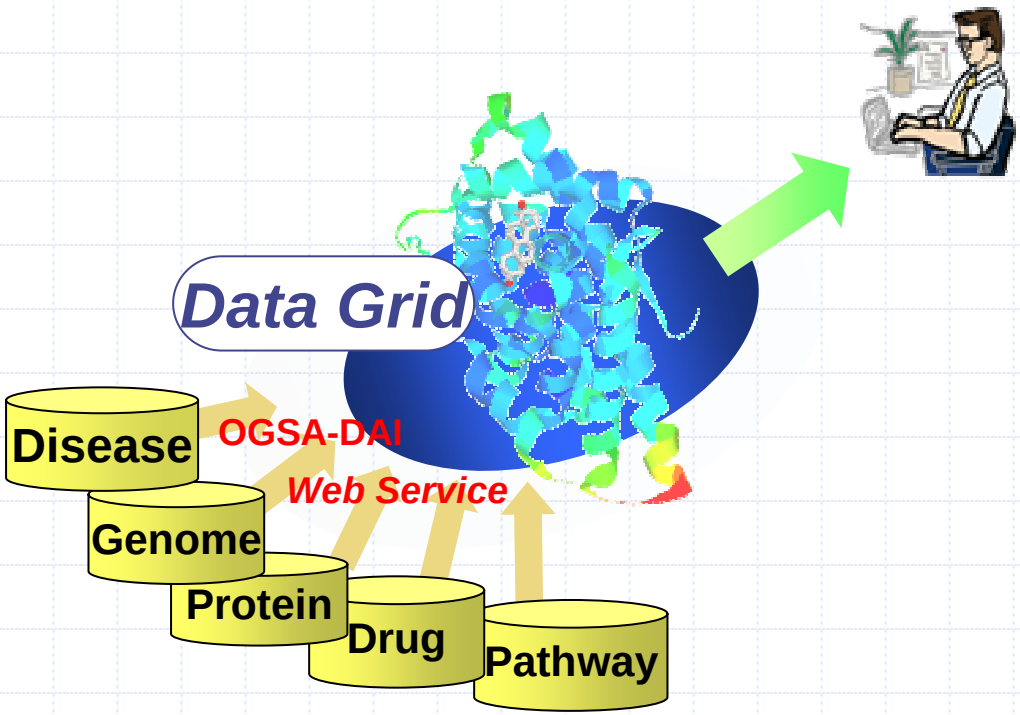
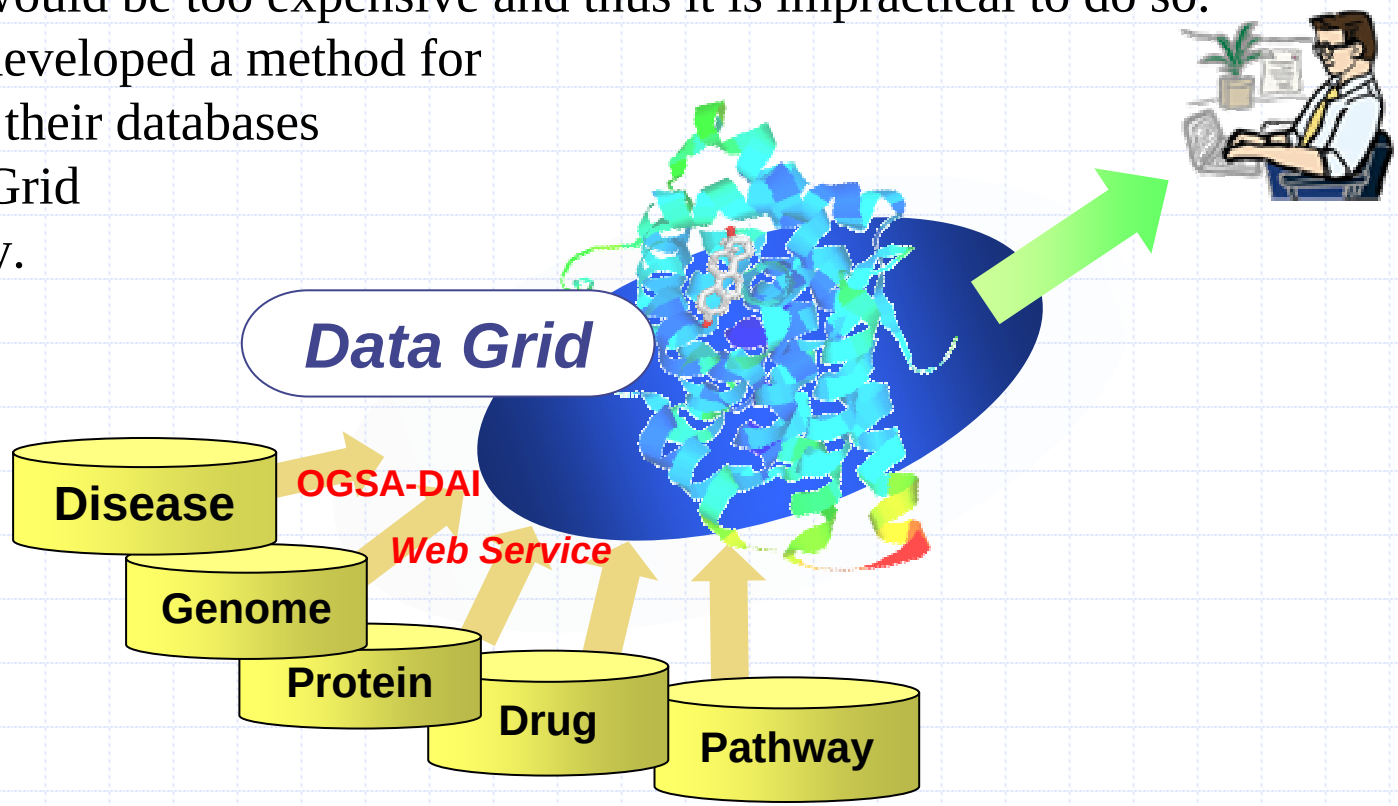
Data Grid Technology Group



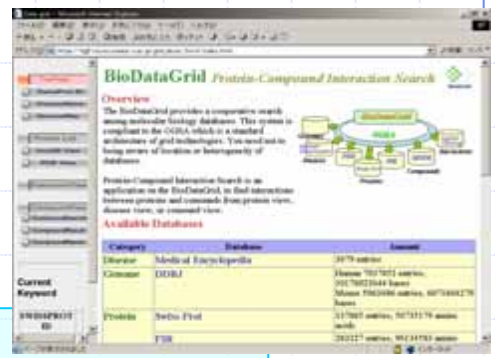
Outline of *DataGrid*

A large number of databases in Molecular Biology and Pharmaceutics exist on web. It is needed to integrate all these databases into one big database for analyzing the entire drug discovery process. However the cost of it would be too expensive and thus it is impractical to do so. We have developed a method for federating their databases using the Grid technology.

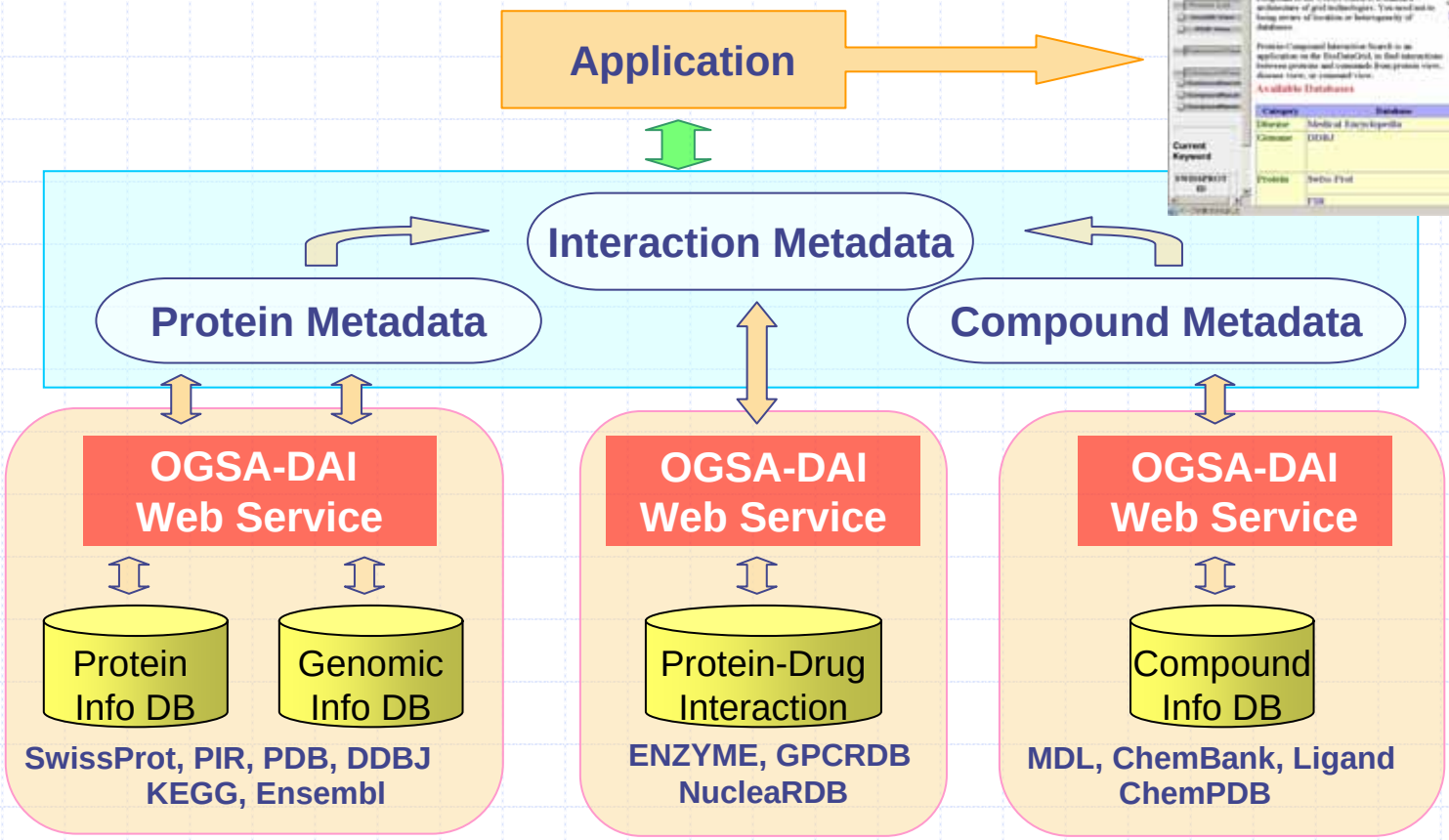


Development of *Data Grid*

Database federation using Grid technology.

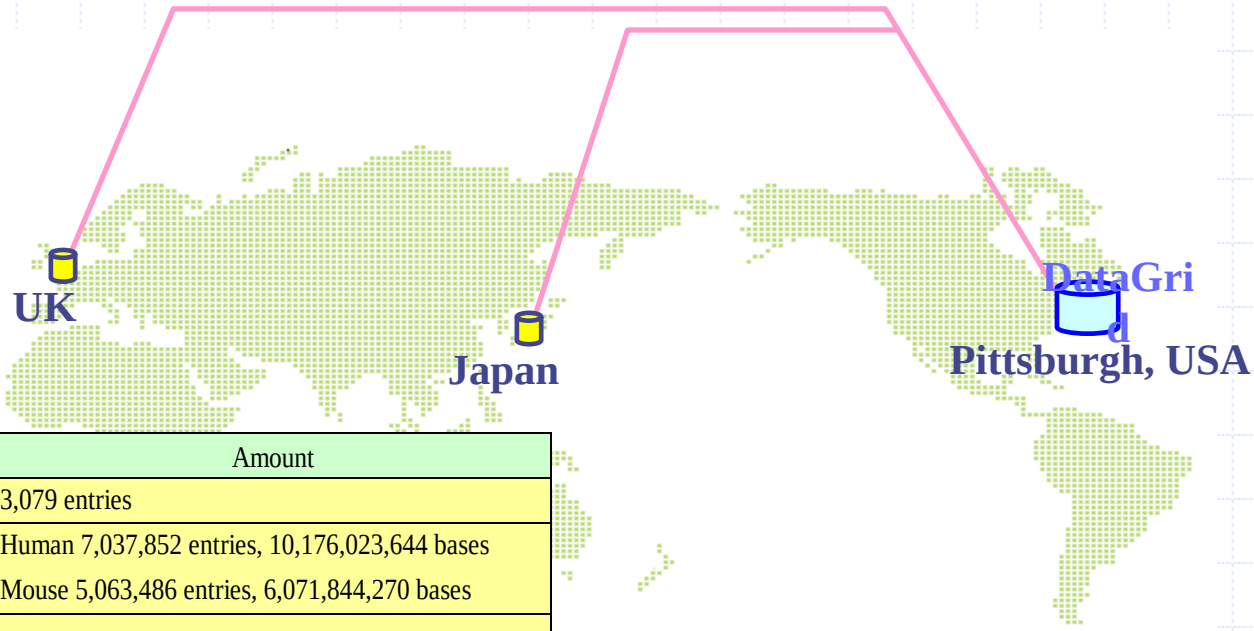


View



Databases for each category are provided as Grid Services

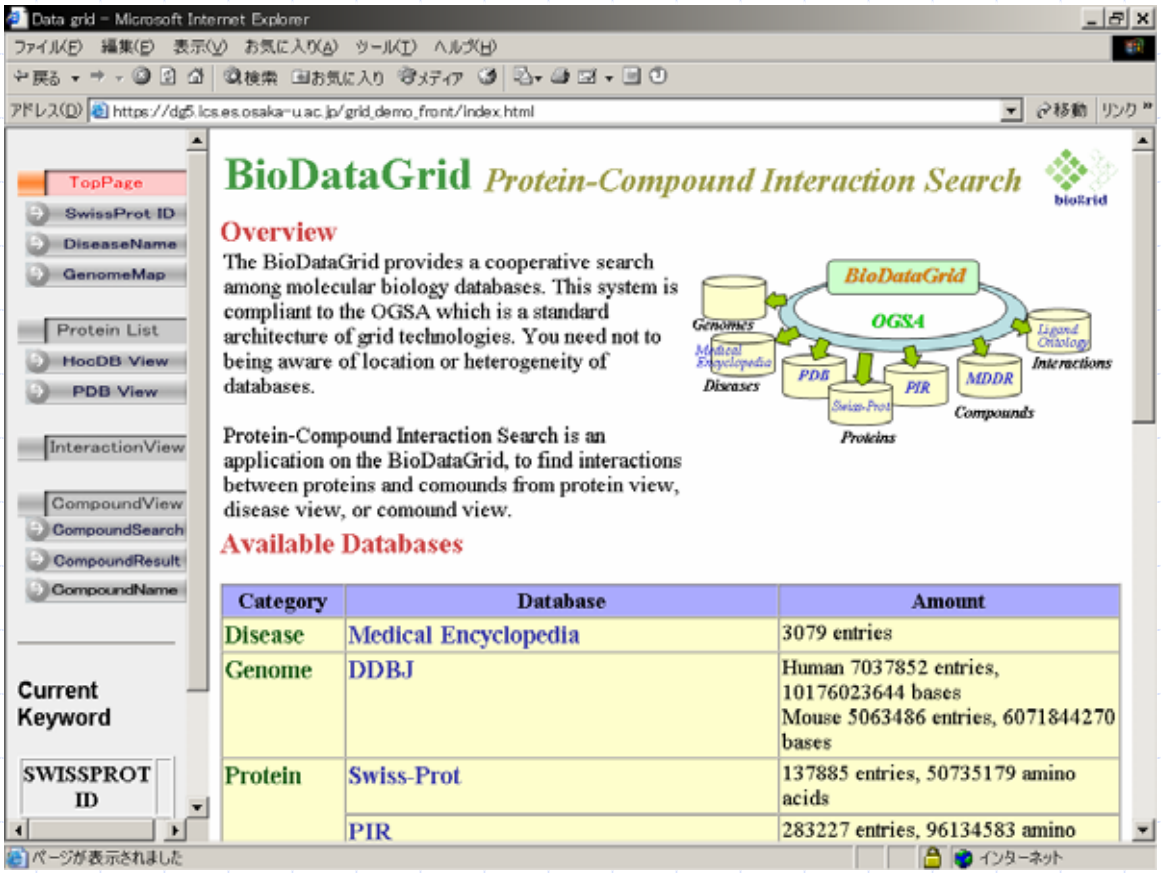
Data Grid system on DBs of the world



Category	Database	Amount
Disease	Medical Encyclopedia	3,079 entries
Genome	DDBJ	Human 7,037,852 entries, 10,176,023,644 bases Mouse 5,063,486 entries, 6,071,844,270 bases
	Ensembl	
Protein	Swiss-Prot	137,885 entries, 50,735,179 amino acids
	PIR	283,227 entries, 96,134,583 amino acids
	PDBj	
	PDB	23,073 entries
Compound	MDDR	14,2553 entries, 9,743 entries
	ChemBank	2,344 entries
	ChemPDB	4,009 entries
	KEGG-LIGAND	11,445 entries for COMPOUND
Interaction	Ligand Ontology	ENZYME, GPCR-DB, NucleaRDB, LGIC-DB

Bio-related databases located at geographically separated sites are federated by our Data Grid system.

Data Grid Application View

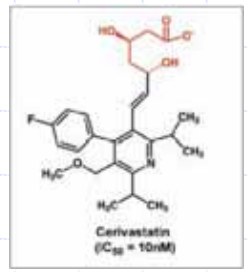


Application Scenario

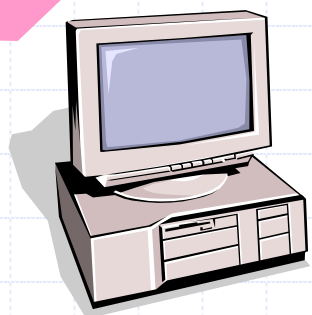
(1)

New Target Protein

Searching for new Ligand by using our Data Grid System



New compounds possibly interacting with the target protein



(2)

In silico Drug Discovery

(4)

(3)

Homologous proteins with known compounds

Large query set of known compounds of homologous target proteins

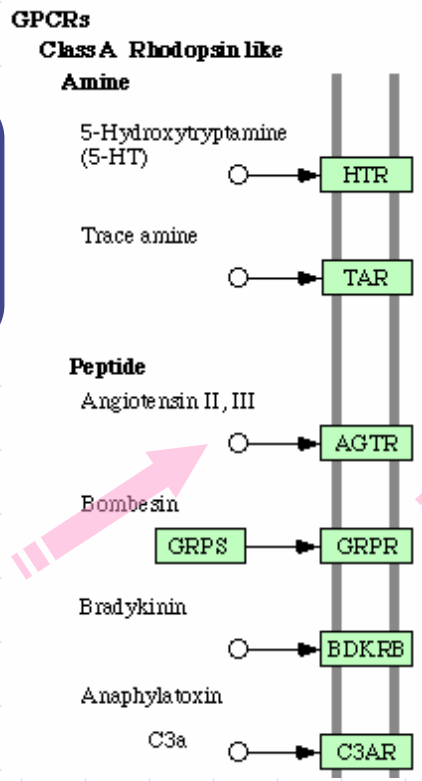
What is new effective drug for adult disease?

We select a new target protein that has been related to the metabolic syndrome, the prevention and treatment of insulin resistance and type2 diabetes.

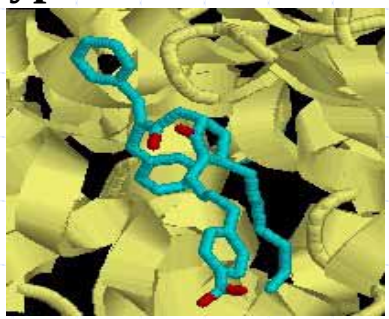
Identify a new Target Protein related to Adult Disease

BLAST Search

Homologous Proteins of the Target Protein



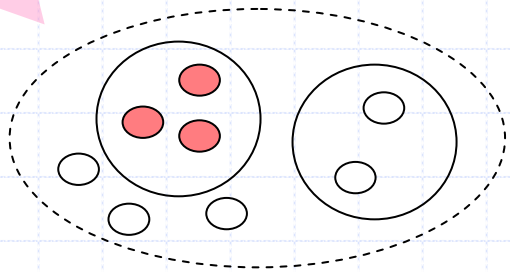
Interaction Search



Telmisartan can function as a partial agonist of PPAR γ
(PDB structure 4PRG)

HIT!!

Compound Similarity Search



Subset of Ligand category

References

1. Schupp, M., et al., *Circulation*. 109(17), 2054-2057, 2004.
2. Farley, S., *Nature Reviews Drug Discovery*. 3(6), 475, 2004.
3. Benson, C.S., et al., *Hypertension*. 43(5), 993-1002, 2004.