Structure-Based Virtual Screening as a Method to Identify Novel Inhibitors of Apical Sodium-Dependent Bile Acid Transporter

Nimish K. Pratha

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NAIST

Research Aims

- Application of PRAGMA network to a virtual-screening problem of current bioinformatic interest
  - Discovery of ligand inhibitor for ASBT (apical sodium-dependent bile acid transporter)

Progress Till Date

- ✓ Identified inhibition sites on ASBT protein
- ✓ Received access to and familiarized self with PRAGMA network and shell interface
- ✓ Installed and began using Chimera, protein preparation program for DOCK
- ✓ Used Chimera to prepare protein files for docking procedure
- ✓ Discussed details of grid machines and available cores with mentor + UF scientists
- ✓ Used Chimera to select docking region spheres
- ✓ Worked with Dr. Ichikawa to set up newly provided cores/VMs
- ✓ Worked with previous students to master DOCK command line and job execution protocol
- ✓ Created docking grid
- ✓ Began transferring files to individual computing nodes
- ✓ Set up initial test jobs
- ~~Start primary batch job~~
  - Technical problems delayed starting
- Resolving technical issues
- Begin to move files to master node in preparation for final job

Progress Goals

- Execution of the full docking job
  - Acquisition of files from ZINC
  - Upload of files to master node

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