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

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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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