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

Progress Goals

- Mobilization of Chimera files to individual computational cores
- Local test run of protein + ligand docking
- Execution of the full docking job

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