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

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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