

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
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- **Start primary batch job**

Progress Goals

- Execution of the full docking job

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