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
Progress Goals

• Completion of Chimera preparation process
• Mobilization of Chimera files to individual computational cores
• Local test run of protein + ligand docking
• Incorporation of new cores (100) to master core list
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