Preliminary Structure and Binding Site Predictions for CCR5 and CXCR4 GPCRs
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CCR5 and CXCR4 are the two main receptors involved in HIV-1 entry into cells. In this project, the transmembrane helices are predicted and then optimized individually. Further work will be done to bundle the optimized helices together and then determine the binding sites for each protein. Various small molecule inhibitors of HIV-1 entry will then be docked to the two proteins. The binding constants for these interactions will be compared to experimental data. The eventual goal of this project is to develop new anti-HIV drugs and to optimize existing inhibitors of HIV-1 entry.