Developing method for predicting binding free energy due to missense mutations

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Abstract: Protein-protein interactions are essential for the function of the cell. If a missense mutation occurs at hot-spots of the binding interface that are crucial in contributing to the interaction, then the binding affinity would be dramatically affected due to geometrical constrains and/or energetic effects. For instance, when substituting a small side chain for a bulky side chain in a narrow binding pocket, the entrance of the partner group will be blocked and the binding process will be completely or partially prevented. Because of that the ability to predict the effect of mutations on the binding free energy is scrucial for revealing the effect of mutations on the cellular function and to predict if the mutations are disease-causing or not.

Method: Ongoing project….