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Alanine Scanning: A computational  
solution to drug design

Computational methods and their application to large systems like proteins have improved vastly in the past few decades. One relatively new computational approach used in drug design is called the alanine scan. An alanine scan determines the stability of proteins and their complexes by comparing the energy changes that occur from amino acid mutations in the protein for alanine. The computational alanine scan provides a much cheaper and quicker alternative to the experimental alanine scanning approach and allows researchers to find mutations that may aid drug design. Like other computational methods, the accuracy of the alanine scan may be called into question. An alanine scan has been run on the chemokine protein, platelet factor 4 (PF4), to determine the stability of a PF4 tetramer. I have optimized this scanning data and found mutations of interest. Actual mutated protein will now be taken and disassociation constants will be obtained experimentally. This experimental test will determine the efficacy and accuracy of the alanine scan performed computationally.



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