Undergraduate Colloquium

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Protein-Protein Docking and the Fast Fourier Transform

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Abstract

Being able to predict how proteins and their ligands or other proteins will interact sheds light on one of the fundamental driving forces of life. Protein-protein interactions play key roles in almost every cell process. For example, understanding these interactions can lead to better disease treatment. A number of the best quasi-rigid-body docking methods cleverly make use of a simple characteristic of the Discrete Fourier Transform, coupled with the speed of a Fast Fourier Transform implementation. This expository talk will present challenges faced in protein-protein docking prediction, as well as the basic algorithms behind a number of rigid-body docking programs, like FTDock and ZDOCK. Finally, some generalizations of the Fourier transform optimized for the problem of protein-protein docking will be discussed.
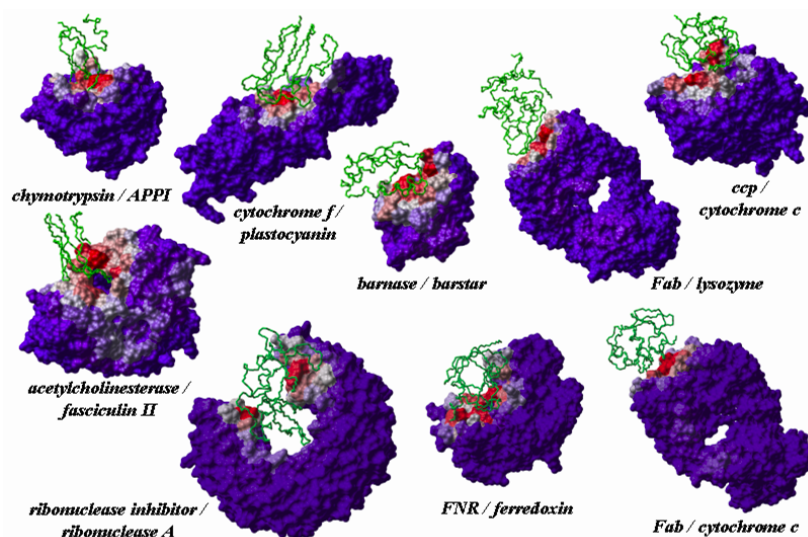
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