Computational Docking and BADock: Predicting Protein Interactions

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Predicting stable protein interactions that may instigate conformational fluctuations to a given amino acid structure is crucial to the advancement of contemporary drug discovery. The capability to precisely foresee interactions allows researchers to propose innovative manners of inhibiting disease processes.

Cutting-edge research nowadays takes advantage of open-source computational "docker" software that permits researchers to effectively screen thousands of molecules and proteins against target proteins. Researchers look for the likelihood of molecules binding or having any interaction at all in chemical space.

The motivation behind this process is elucidated in the subsequent example. Let's assume we aim to find a drug to cure Parkinson's disease. We recognize that it is caused by an aggregation of misfolded proteins. If we could find a small molecule, computationally, to bind a reactive pocket or region of our protein, we may cause a conformational change in that protein. This is to say that the small molecule would bind and then the protein would switch it's folding conformation back to the "wild-type" (regular) conformation. If this were the case, imagine the implications computational drug discovery could have!

So let's introduce BADock, an open-source docking software that forecasts interactions between any two given amino acid structures. Unlike many other docking programs, the user does not need to pass in an input that explains how the protein is folded. BADock can output stability of interactions between proteins that may or may not have known folding patterns. This is a revolutionary new open-source software! The ability to predict protein-folding is a problem within itself, let alone trying to find the interactions between two unknown protein structures.

The usage of this software is multi-fold! Based on competitor docking programs and experimental data, these researchers were able to show that their predictions had high real-world accuracy. To read more about the results and implications of this research, look at the official paper from *Bioinformatics*.