Controlling Protein Activity with Conformational Switches

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In my research project, our focus centered around being able to control the activity of a movement-regulating protein (known as CheY) by inserting a guiding protein switch (known as UniRapR) that was created. The idea is to get UniRapR, both affected by a drug and without a drug, to take over the dynamics of CheY – in a sense, allowing us to control the protein complex. These simulations are done computationally (in silico, aka in the computer).

This work matters because the ultimate end goal at the completion of this research is to be able to target and control diseases cells in the human body (such as cancer, HIV, etc) in order to stop them from replicating and/or spreading. Of course, it is important to note that this project was a very preliminary first step to reaching that goal, and further testing will be done (in vitro, aka in cells).
Results

- The results of my project came in the form of data that was created via the protein simulations. Basically, the protein complexes gave root-mean-square deviation (RMSD) values which represent the dynamics of the protein, and the activity essentially showed that the dynamics of CheY (as a control) is very similar to the dynamics of when it is switched by the drug-affected UniRapR.

- These results are important to the research community (on behalf of this project as a whole) because they provide the basis of support behind the first step towards designing drug-controllable switches.

- These results are important to the general audience because, as aforementioned, they represent the preliminary work that will hopefully (in the future) allow us to control diseased cells in the human body in order to stop diseases in their tracks.

In this graph, the black dots represent CheY, which is the control. The red dots represent UniRapR without drug-induction, and the green dots represent UniRapR with drug-induction. As shown, the dynamics of the UniRapR that is drug-affected correlates more with the control (CheY). This lets us know that drug-controllable switches are feasible for further research to be done of them so that they can be implemented.