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by

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## ***Predicting the Breaking Order of Contacts during Protein Stretching***

### *ABSTRACT*

Mechanical stretching of proteins (e.g. in muscles) is one of the most important, a yet not fully understood problems in biology.

It has been shown that a coarse grained Go-like model is sufficient to reproduce experimental data obtained from atomic force microscopy AFM. This model has significant computational advantages over all atom simulations, especially for large and complex structures.

Elastic properties of proteins can be well described by a simple Gaussian Network Model (GNM), that predicts very well crystallographic B-factors.

Our goal is to combine both methods to predict behavior of proteins under external stretching. We have studied four proteins: 1tit, 1ubq, 1crn) and a 1aua.

First we stretched proteins by performing dynamics simulations with the Go-like model. From this we obtained the force-displacement curves and scenarios of possible mechanical unfolding. We used the GNM model to calculate B-factors and the slowest modes of motion for the stretched proteins and compared them with the predicted order of breaking contacts between residues in the Go-like model. Using the GNM we identified the hinge points - the residues where the force is the strongest. Contacts between those residues usually break first with the increase of the external force.

We found that for 1tit and 1aua the order of the contact breaking is very well predicted but for 1ubq and 1crn is (at the moment) less satisfactory.

We anticipate that this method can be a powerful new tool to understand stretching of even more complex systems like the Holliday junctions in DNA.