Model unfolds proteins gently

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Protein molecules inside cells are constantly reorganizing themselves, driven by very tiny forces exerted by all the other molecules in their crowded environment. Most experimental techniques and theoretical/computational models are necessarily built around much greater driving forces. A new theoretical model reported in the *Journal of Chemical Physics* investigates the unfolding of fibronectin under gentler conditions.

"Typical models study very fast processes and consume a lot of CPU time," says author Alessandro Pelizzola of the Politecnico di Torino in Italy. "The strengths of our model are simplicity and the ability to model the slow, low-force processes that actually occur inside the cell."

Under the smaller forces, the researchers discovered a previously uncharacterized sequential loss of structure involving a fluctuation between two intermediates of similar complexity. The unfolding was demonstrated to involve many more steps than previously shown in experiments and more complex models. Because the model probes forces that are an order of magnitude smaller than those currently available to experimentalists, it can lead to a better understanding of biomolecular transitions within the cell.

"These small forces are beyond the current experimental techniques" says Pelizzola, "but I would expect the experiments to be possible in a few years." The model has been applied to other biomolecular processes with similarly detailed results.

More information: The article, "Pathways of mechanical unfolding of FnIII10: low force intermediates" by M. Caraglio, A. Imparato, A. Pelizzola appears in The *Journal of Chemical Physics*. link.aip.org/link/jcpsa6/v133/i6/p065101/s1

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