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Observing Stepwise Unzipping of Neuronal Snare Protein with Steered Molecular Dynamics MUSTAFA TEKPINAR, Yuzuncu Yil University, WENJUN ZHENG, University at Buffalo — Soluble N-ethylmaleimide-sensitive factor Attachment Protein Receptors (SNARE) play a crucial role in membrane fusion. Neuronal SNAREs are made up of four helices: a snaptobrevin, a syntaxin 1, and two SNAP-25 helices. We applied constant velocity pulling forces to C terminal of snaptobrevin in SNARE complex to understand unzipping mechanism of neuronal SNAREs. We successfully observed unzipping of snaptobrevin from the other three helices in two steps: C terminal unzipping and N terminal unzipping. Our results have good agreement with recent optical tweezer experiments that observe this stepwise unzipping. Additionally, our simulations reveal that these two steps differ from each other. We believe that these different mechanisms can help us to understand SNARE mediated membrane fusion process better.

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