Botulinum Neurotoxin: Unique Folding of Enzyme Domain of the Most Poisonous Poison

Supporting Material

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*Running Title: Unique Folding of BoNT/A Light Chain

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Figure S1. Secondary structure dynamics of the BoNT/A in urea solution from MD simulations at 25 °C. Shown are the secondary structure propensities of various residues as a function of time. Color denotation for α-helices, β-sheets, and random coil is presented in the graph (turns, 3_{10}-helices, and π-helices are shown in blue, red and gray color, respectively).
Figure S2. Tertiary structure dynamics of the BoNT/A in urea solution from MD simulations at 25 °C. Shown are the profiles of the structure overlap $\xi$ as a function of time (see Experimental Methods in main text).
Figure S3. ANS (8-anilino-1-napthalene sulphonic acid) binding to urea denatured BoNT/A LC at room temperature (25 °C). Here, $I_{488}$ is the measured fluorescence emission intensity of ANS at $\lambda = 488$ nm after exciting the solution at $\lambda = 388$ nm. ANS is a dye which binds to hydrophobic residues of a protein molecule. In this experiment, 70 µM of ANS was titrated into 1 ml of 1 µM solution of BoNT/A LC dissolved in 10 mM sodium phosphate buffer (pH = 7.4), containing 50 mM NaCl, 1 mM DTT, and urea at the required concentration in a 1 cm path-length cuvette.