

Abstract Submitted  
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**Polymorphic Ab protofilaments exhibit distinct conformational dynamics as calculated by normal mode analysis** MATTHEW ARMBRUSTER, PATRICIA SOTO, Creighton University — This project proposes to test the hypothesis that the physicochemical milieu modulates the conformational dynamics of synthetic Alzheimer's Ab protofilament structures, the main component of Alzheimer's senile plaques. To this end, 3D solid-state NMR structures of Ab protofilaments were used as initial structures for molecular dynamics simulations in explicit water and a water/hexane environment. The initial structures of the simulations and representative structures from the simulation-generated trajectories were taken to perform computational normal mode analysis. We developed a code in python with a graphical user-friendly interface. The program incorporated the ProDy (0.7.1) package. With the application, we examined cross-correlation plots of Ca positions of the 2-fold Ab protofilaments along the most collective mode and the slowest mode. The protofilament structures were highly correlated in the water environment. We hypothesized the protofilament would move as one in water because of the viscosity. The square fluctuation of Ca positions was calculated for the slowest mode for the hexane model and the MD generated ensemble. The two plots match up until midway through the structure. At the midway point a phase shift emerged between the two structures most likely where the surrounding changes. The in-house developed code made it easy to perform analysis and will be used by other students in the research group.

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