

Effects of zinc on beta amyloid dynamics

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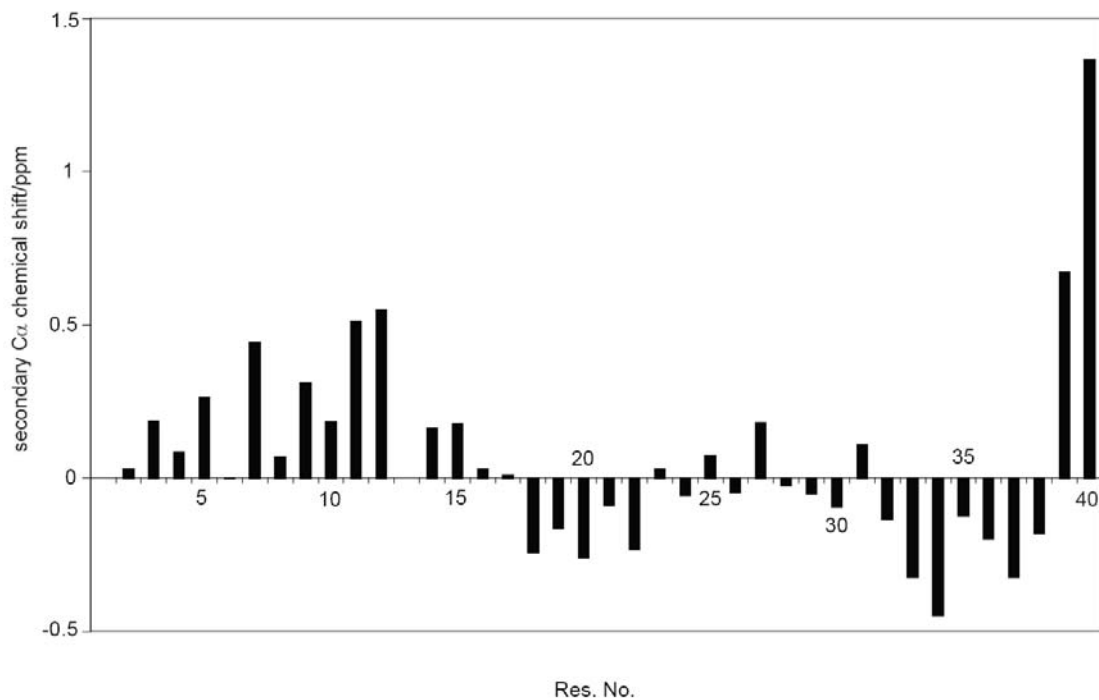


Fig S1. Secondary carbon alpha ($C\alpha$) chemical shifts of $A\beta_{40}$ in the zinc-free form. Residues 18-22 and Gly29 toward C-terminus reveal a tendency for an extended conformation, while the intervening residues of 23-28 adopt a less extended conformation. The random coil values were predicted by CamCoil (De Simone et al., 2009) using a pH of 6.1, and average values over a window of three residues are shown here.

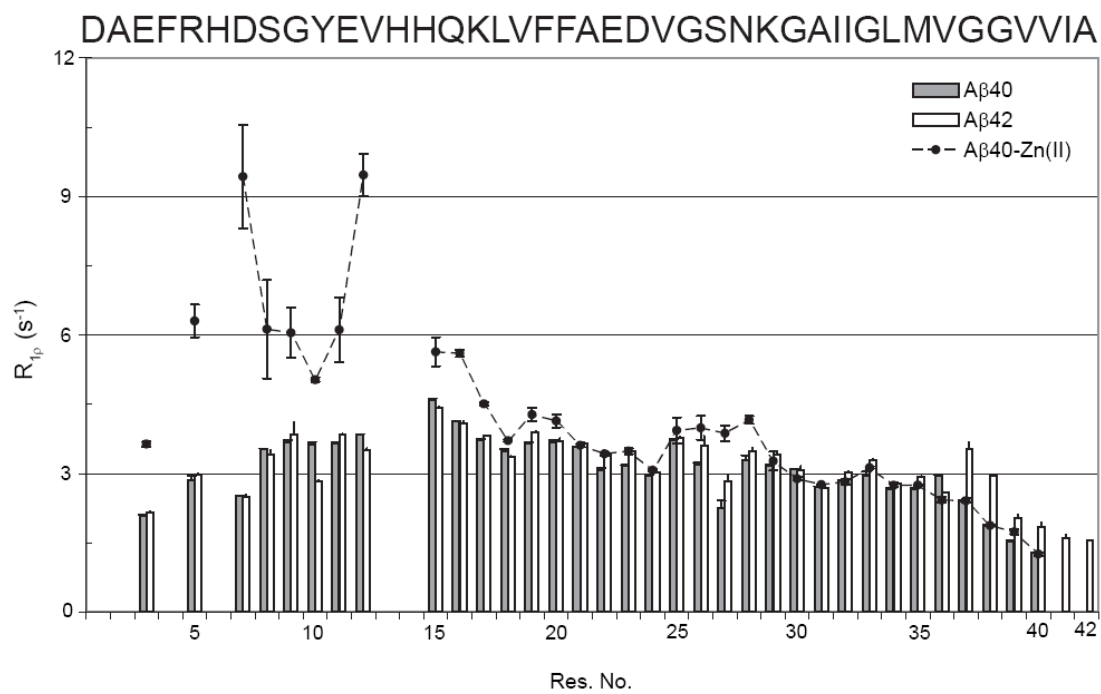


Fig S2. ^{15}N $R_{1\rho}$ relaxation rates for A β 40 in the absence or presence of equimolar zinc and A β 42.

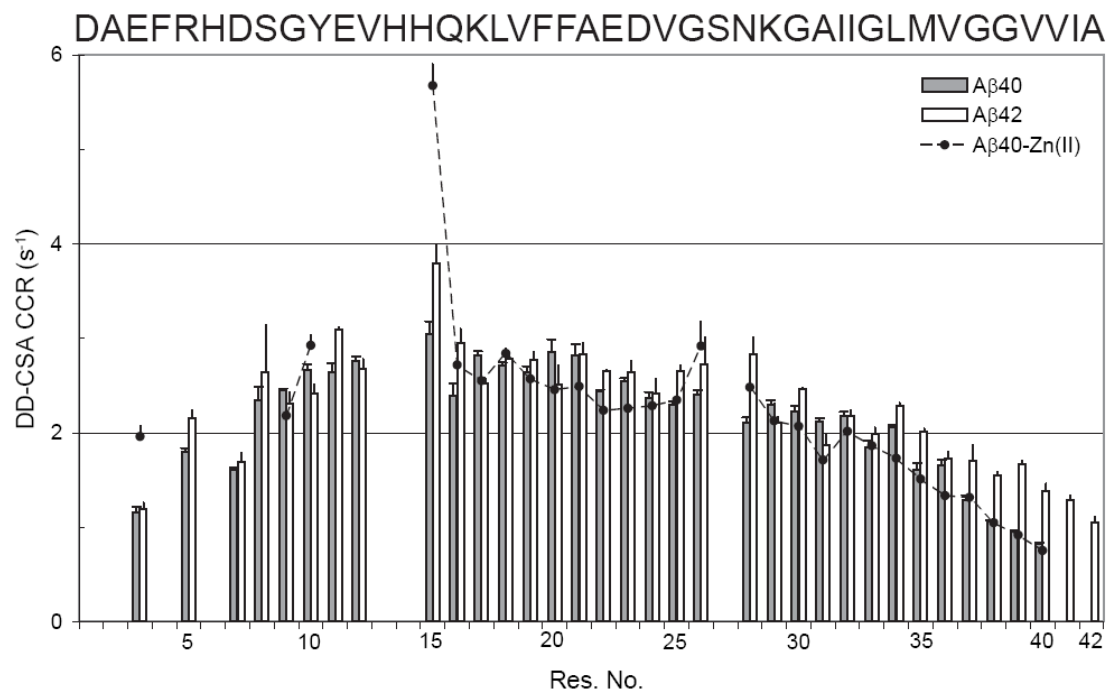


Fig S3. Cross-correlated relaxation rates (CCR) between ¹H-¹⁵N dipole-dipole (DD) and ¹⁵N chemical shift anisotropy (CSA) relaxation mechanisms, measured for Aβ40 in the absence or presence of equimolar zinc and Aβ42.

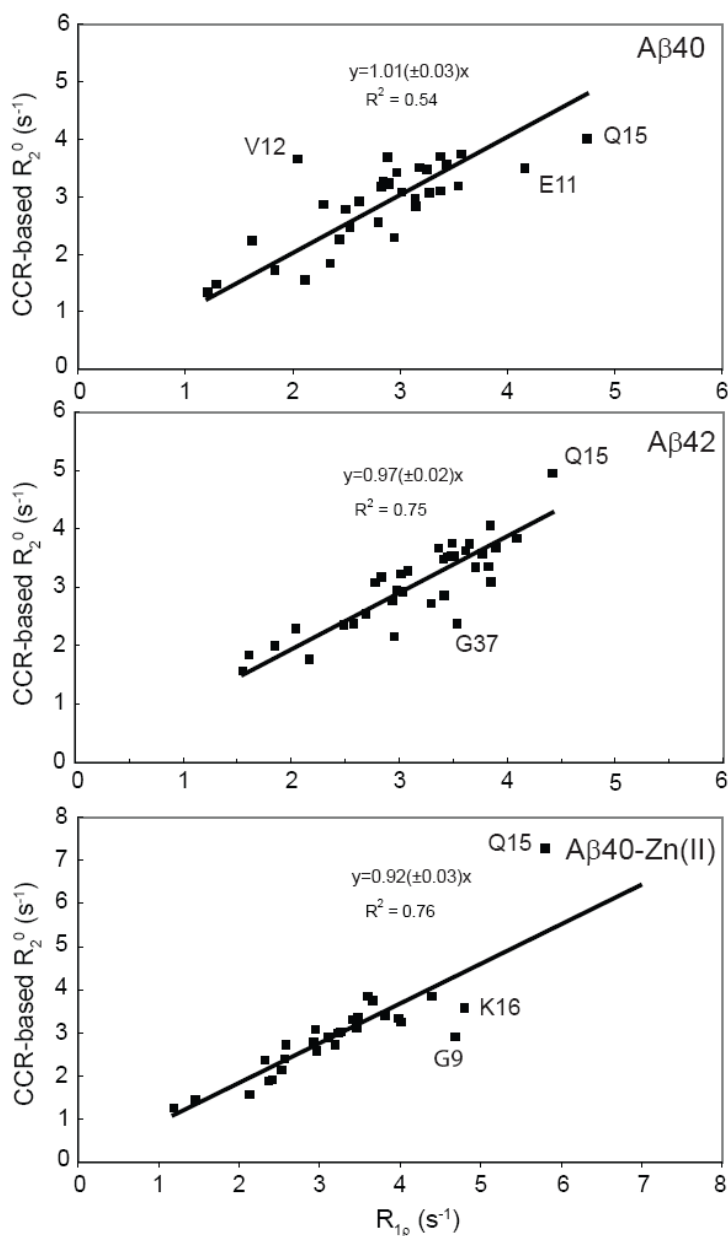


Fig S4. Correlation between ^{15}N $R_{1\rho}$ and cross-correlated relaxation rate (CCR)-based exchange-free transverse relaxation rates, for A β 40 in the absence or presence of equimolar zinc and A β 42. The slopes less than 1 for zinc-bound A β 40 and A β 42 reveal that the exchange contribution is not fully eliminated from the $R_{1\rho}$ data. Some of the peaks with significant deviation from the fitted line have been marked, and they are all located in or close to the binding region.

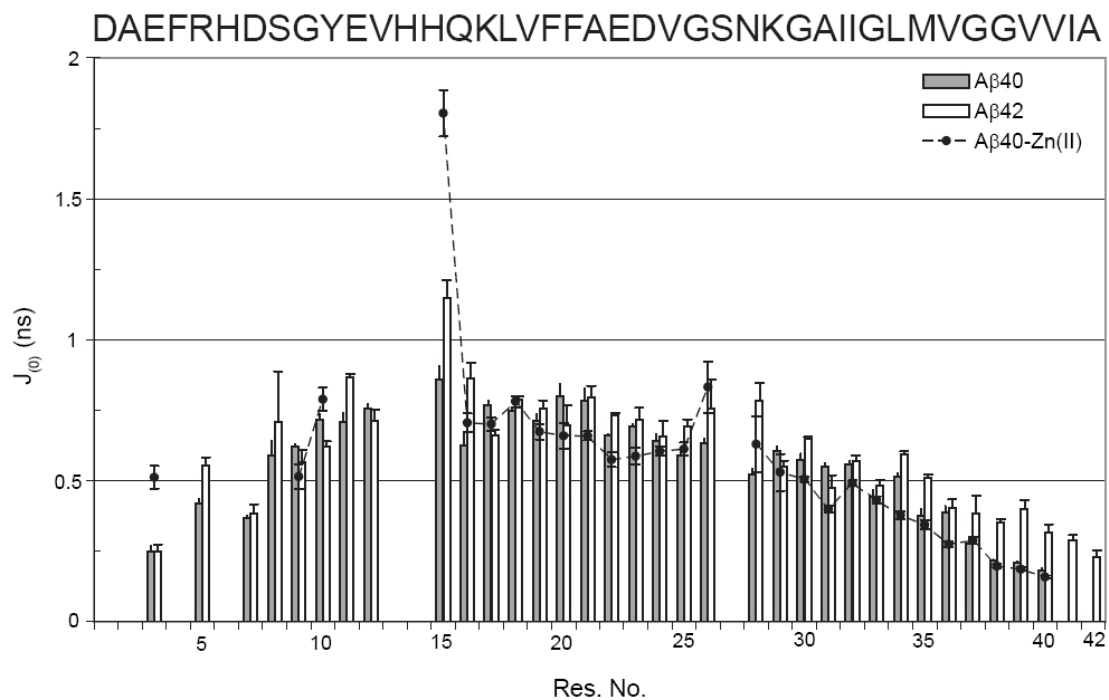


Fig S5. Spectral density function at frequency 0, $J(0)$, calculated through reduced spectral density mapping using ^{15}N R_1 , CCR-based exchange-free R_2 and ^1H - ^{15}N heteronuclear NOE values for A β 40 in the absence or presence of equimolar zinc and A β 42. Larger values of $J(0)$ indicate higher rigidity on a time scale comparable to the correlation time. Difference values are shown in Fig. 5B.