Supporting Information

A Network of Conformational Transitions Revealed by Molecular Dynamics Simulations of the Carbonic Anhydrase II Apo-enzyme

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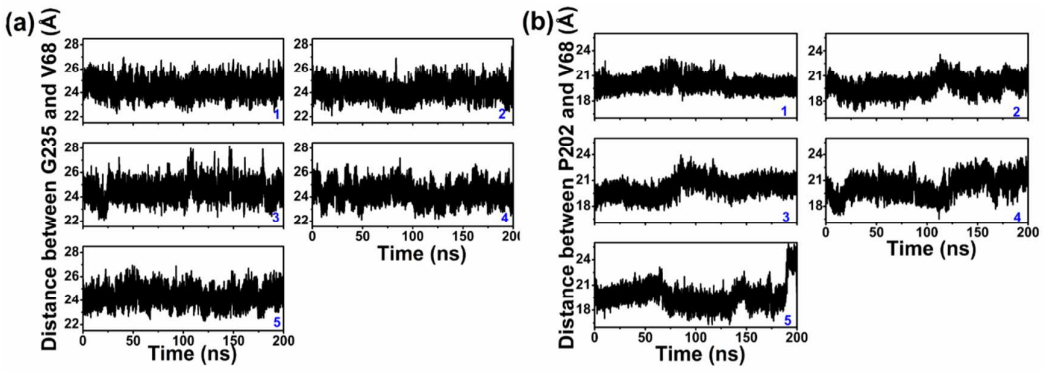

Figure S1. The time evolution of the Cα distances between Pro202 and Val68 (a) and between Gly235 and Val68 (b) in the MD trajectories.

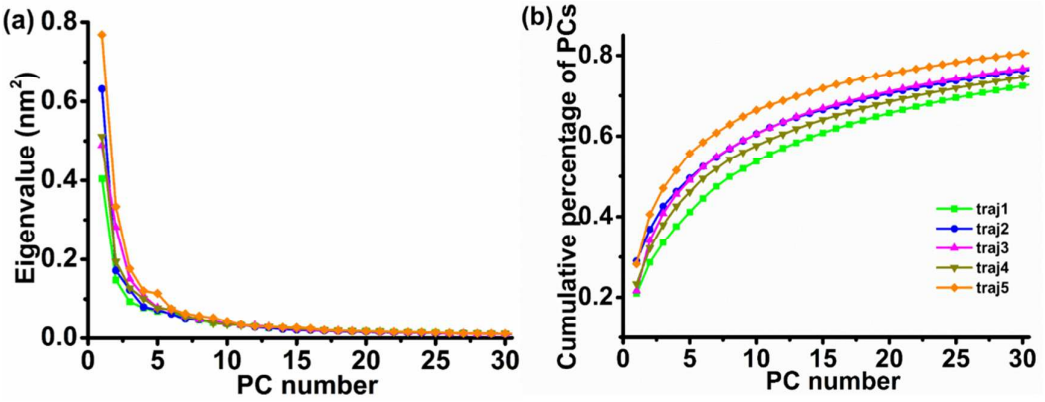

Figure S2. The magnitudes (a) and cumulative percentages (b) of the first 30 PC eigenvectors of the MD trajectories.

$$\begin{bmatrix} 1.0 & -2.9e-5 & -7.2e-5 & 2.2e-5 & -5.4e-5 & -2.3e-5 & -3e-6 & 8e-6 & -1.5e-5 & 2e-5 \\ -2.9e-5 & 1.0 & -9e-6 & 9.7e-5 & -2.8e-5 & -2.8e-5 & 5e-5 & 3.2e-5 & 3.4e-5 & -5.9e-5 \\ -7.2e-5 & -9e-6 & 1.0 & 4.5e-5 & 5.1e-5 & 6.7e-5 & 2e-6 & 4.8e-5 & -3.4e-5 & 3.7e-5 \\ 2.2e-5 & 9.7e-5 & 4.5e-5 & 1.0 & -4.1e-5 & -3.8e-5 & -5e-5 & -2.3e-5 & 1.3e-5 & 3e-5 \\ -5.4e-5 & -2.8e-5 & 5.1e-5 & -4.1e-5 & 1.0 & 9e-6 & -7e-5 & 2e-6 & 4.8e-5 & -9.6e-5 \\ -2.3e-5 & -2.8e-5 & 6.7e-5 & -3.8e-5 & 9e-6 & 1.0 & -6e-5 & 4.6e-5 & 5.4e-5 & 5.7e-5 \\ -3e-6 & 5e-5 & 2e-6 & -5e-5 & -7e-5 & -6e-5 & 1.0 & -2.7e-5 & 1.5e-5 & 2e-6 \\ 8e-6 & 3.2e-5 & 4.8e-5 & -2.3e-5 & 2e-6 & 4.6e-5 & -2.7e-5 & 1.0 & -1.1e-5 & -4.6e-5 \\ -1.5e-5 & 3.4e-5 & -3.4e-5 & 1.3e-5 & 4.8e-5 & 5.4e-5 & 1.5e-5 & -1.1e-5 & 1.0 & 4.3e-5 \\ 2e-5 & 3.7e-5 & 3.7e-5 & 3e-5 & -9.6e-5 & 5.7e-5 & 2e-6 & -4.6e-5 & 4.3e-5 & 1.0 \end{bmatrix}$$

Table S1. The inner products of the eigenvectors of the first 10 PCs, which are represented as a 10×10 matrix.

Table S1 shows that: The inner products of the same eigenvectors are nearly 1, which means the eigenvectors of every PCs are normalized; and the inner products of the

different eigenvectors are nearly 0, which indicates these eigenvectors are orthogonal and have no correlation with each other. Therefore, the PCA is valid for our study.