Supporting information for:

Conformational Heterogeneity in the Michaelis Complex of Lactate Dehydrogenase: An Analysis of Vibrational Spectroscopy Using Markov and Hidden Markov Models

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Figure S1: Box plot of the distributions of the minimum distances between carbonyl oxygen of pyruvate and active site residues in (a) the X-ray structure state $S_{\text{xray}}$, (b) the flipped state $S_{\text{flip}}$, (c) the rotated state $S_{\text{rotate}}$, and (d) the associated/unbound state $S_{\text{a/u}}$. 
Figure S2: Box plot of the distributions of the minimum distances between carboxyl oxygens of pyruvate and active site residues in (a) the X-ray structure state $S_{\text{Xray}}$, (b) the flipped state $S_{\text{flip}}$, (c) the rotated state $S_{\text{rotate}}$, and (d) the associated/unbound state $S_{\text{a/u}}$. 
Figure S3: Box plot of the distributions of the minimum distances between methyl carbon of pyruvate and active site residues in (a) the X-ray structure state $S_{\text{ray}}$, (b) the flipped state $S_{\text{flip}}$, (c) the rotated state $S_{\text{rotate}}$, and (d) the associated/unbound state $S_{\text{u/u}}$. 
Figure S4: Implied relaxation timescales as a function of lag time for (a) the MSM estimated from the microstates on the basis of the substrate binding only, (b) the MSM estimated from the microstates on the basis of the protein conformations as well as the substrate binding, and (c) the coarse-grained kinetic model (hidden Markov model) estimated from the same microstates as in (b).
Figure S5: Output probabilities from hidden to observable discrete states.