

Figure S3. Comparison of power spectral density functions of EMD and TMD<sub>1</sub> simulations. Power spectral density per residue (or residue-averaged MSF) for (A) WPD loop, and (B) residues on which TMD potential was not directly applied. Frequency components of EMD and TMD<sub>1</sub> simulations are represented with black and blue solid lines, respectively. Gray and yellow dashed lines represent the least-squares lines fit to EMD and TMD<sub>1</sub> data, respectively. Base frequency and the upper harmonics (peaks) are more clearly seen in the  $C_{\alpha}$  atomic trajectory spectrum of the WPD loop. Existence of peaks in the power spectrum of regions on which TMD potential was not directly applied shows that effects of local disturbance propagated to the rest of the protein.