Supporting Information

Path Ensembles for Pin1-catalyzed Cis-trans Isomerization of a Substrate Calculated by Weighted Ensemble Simulations

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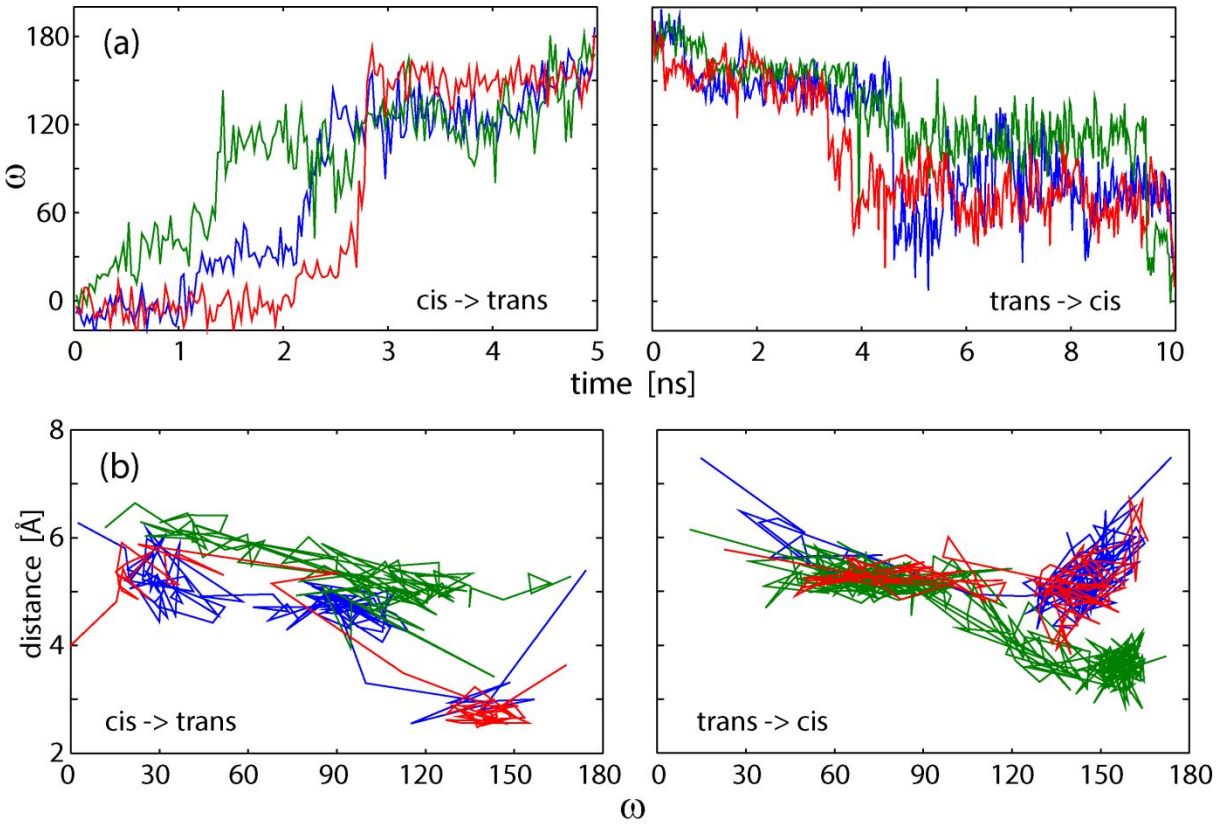

Figure S1.

Three representative paths obtained from the WE simulations of both cis → trans (left) and trans → cis (right). (a) ω as a function of the simulation time, and (b) two-dimensional plots along ω and the atom distance between Ser154O_γ and pSerO of the substrate (see Fig. 4a).

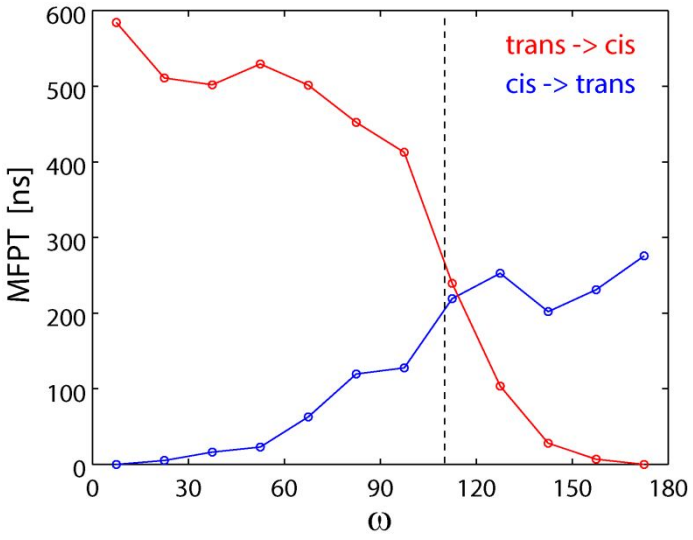

Figure S2.

Mean free passage time (MFPT) as a function of ω, calculated from the WE simulations of both cis → trans (blue) and trans → cis (red).