

Theoretical Study on Signal Transduction Process of Bacterial Photoreceptor PpSB1 Based on Markov State Model

Yajie Zhao ^a, Yue Zhang ^a, Minzhang Sun^a and Qingchuan Zheng ^{a, b*}

^a Laboratory of Theoretical and Computational Chemistry, Institute of Theoretical Chemistry, International Joint Research Laboratory of Nano-Micro Architecture Chemistry, College of Chemistry, Jilin University, Changchun 130023, People's Republic of China

^b Key Laboratory for Molecular Enzymology and Engineering of the Ministry of Education, Jilin University, Changchun 130023, People's Republic of China

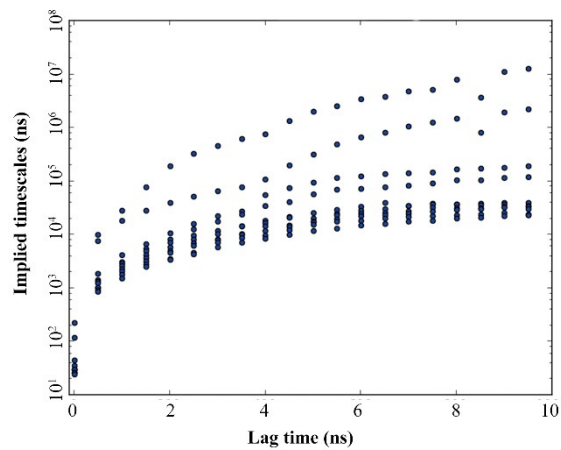


Figure S1. Markov state models of PpSB1-LOV domain. A plot of the implied time scales for a series of 161 microstate Markov state model built at lag time from 1 to 20 ns. The slowest time scales level out around 4 ns, which indicated the model was Markovian. The lag time was selected for the microstate model. The implied time scales suggested that there were 3 slowly processes. Thus, the higher resolution MSMs with five states would be constructed.

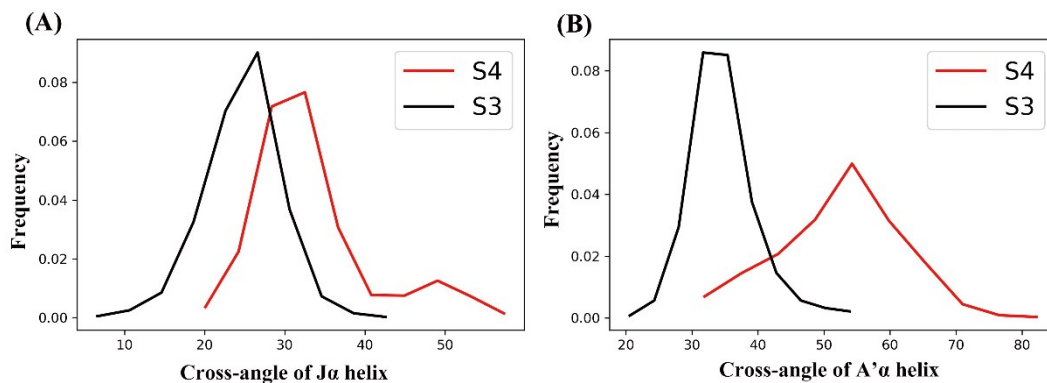


Figure S2. Increase of the cross-angle of $J\alpha$ and $A'\alpha$ helices in the S3 and S4, respectively. (A) $J\alpha$ helix. (B) $A'\alpha$ helix.