Supporting Information

In this research, five independent trajectories were simulated for P480 and P500* states and the RMSDs cannot be identical due to different initial speeds. The RMSD curves (Figure S1) display that both P480 and P500* states reach equilibrium at the last 50 ns (except No. 1 trajectory of P500*, as seen in Figure S1b). As for the distances in Figure S2, we calculated the average value of distances of $RSBH^+$-D253 and $RSBH^+$-E123 respectively for the No.2 ~No.4 trajectories, and selected the No. 4 trajectory to analyze.

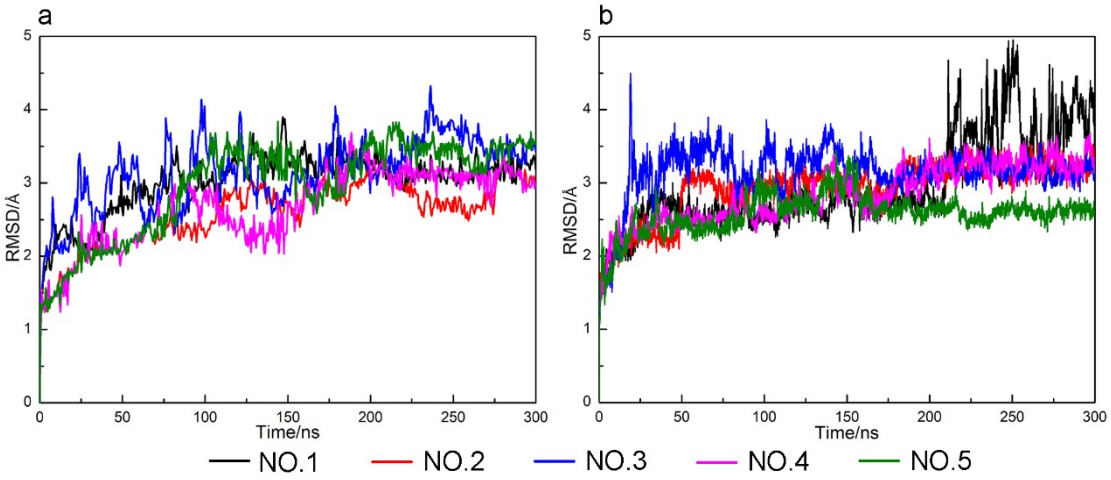

Figure S1. RMSDs of five independent trajectories for (a) P480 state and (b) $P500^*$state.

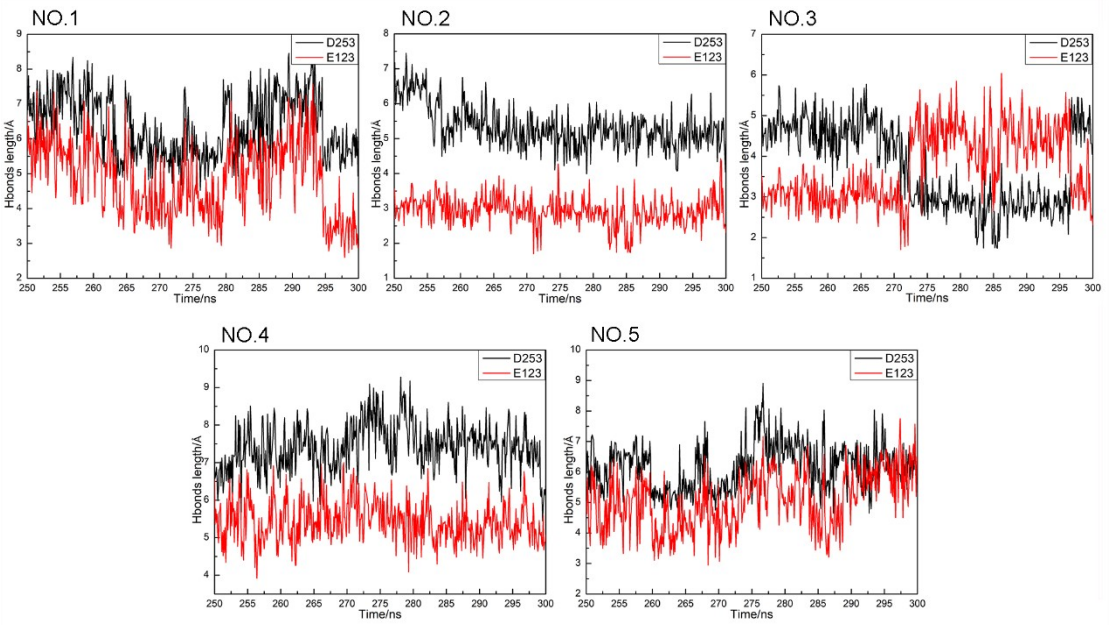

Figure S2. The distances between $RSBH^+$ and counter residues (E123 and D253) of P500* state in the last 50ns for each trajectory.

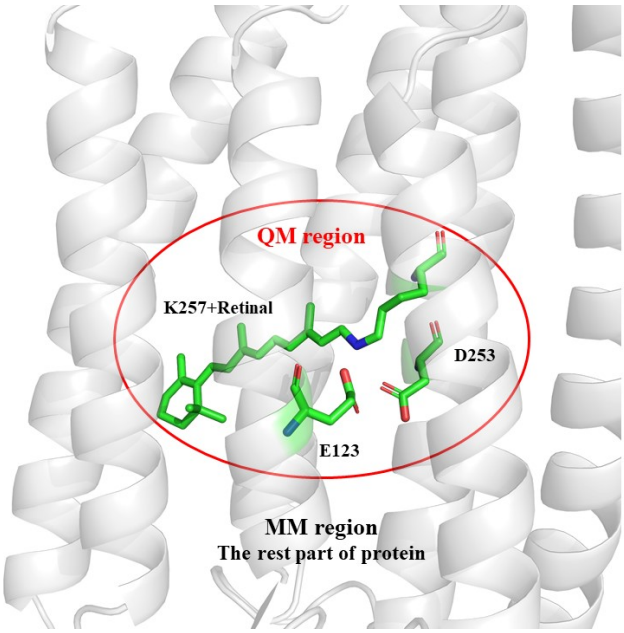

Figure S3 Scheme of QM and MM regions.

Table S1. The probability of $RSBH^+$ forming hydrogen bonds with E123 and D253 in each simulation.

	NO.1	NO.2	NO.3	NO.4	NO.5
D253	0	0	0	0	0
E123	6.4%	4.8%	6%	0	0.8%