Design of RuBP Derivatives for the Modulation of Carboxylase Specificity

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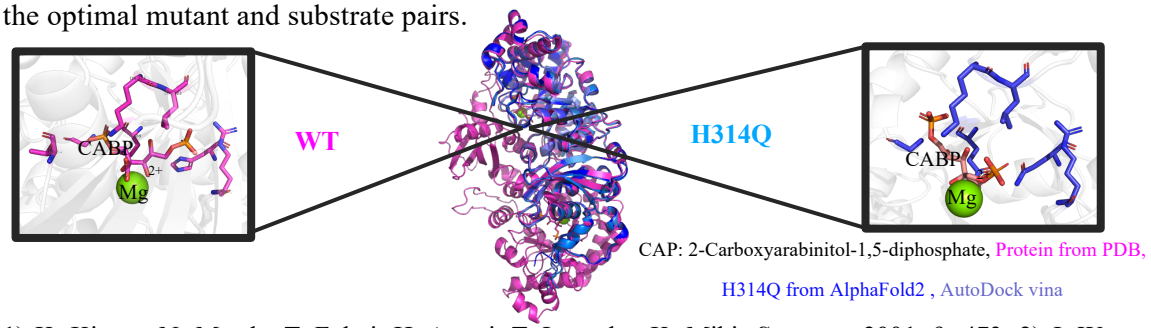
Ribulose-1,5-bisphosphate carboxylase/oxygenase (RuBisCO) is the most abundant enzyme on Earth. RuBisCO plays a key role in achieving carbon neutrality by facilitating the reduction of atmospheric CO_2 accumulation. While RuBisCO has a low catalytic capacity and turnover rate for its specific natural substrate, ribulose 1,5-bisphosphate (RuBP), its cofactor-independent carbon fixation reaction makes RuBisCO an attractive candidate for further engineering. This research aims to extend the CO_2 fixation ability of *Tk*-RuBisCO with substrates other than RuBP.[1,2]

In silico experiments and predictions of *Tk*-RuBisCO (*Thermococcus kodakarensis* RuBisCO[3]) demonstrated its thermostable properties, raising the possibility of introducing multiple mutations while maintaining the ability to correctly fold and retain the predicted structure[4]. Docking results indicated a disruption of hydrogen bond formation between RuBP derivatives and candidate mutants at the active sites. Further efforts are underway to identify the optimal mutant and substrate pairs.



CAP: 2-Carboxyarabinitol-1,5-diphosphate, Protein from PDB, H314Q from AlphaFold2 , AutoDock vina

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