Rational design engineering of a thermostable α- carbonic anhydrase from Sulfurihydrogenibium yellowstonense to improve its thermostability for industrial applications

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Abstract

Carbon dioxide (CO2) capture and storage (CCS) processes could benefit from thermostable carbonic anhydrases (CAs), which can significantly increase the rate of CO2 absorption into solvents. Since conventional CO2 absorption techniques are usually performed under high-temperature conditions in industrial plants, implementing highly thermostable CAs is very important to introduce a robust and economical process. The present study employed a combination of in silico tools to rationally engineer a thermostable CA (SspCA) originating from a thermostable bacterium Sulfurihydrogenibium yellowstonense. Based on the results, while the general folding of the enzyme and its catalytic efficiency was retained in the K100G mutant, the melting temperature increased by 3°C, and the CO2 hydration activity half-life at 85°C increased by two times. Molecular dynamics (MD) simulations were performed to determine the underlying causes of the thermostability improvement. The K100G mutation was shown to cause a reduction in protein local flexibility mainly by confining the flexible parts due to rearrangement of salt bridges and hydrogen interactions network. In sum, while strengthening the importance of rational design in thermostable enzymes, the present study showed the capability of merely one rationally-designed mutation which indirectly resulted in CA thermostability improvement by exerting local structural rigidification in its neighboring part.

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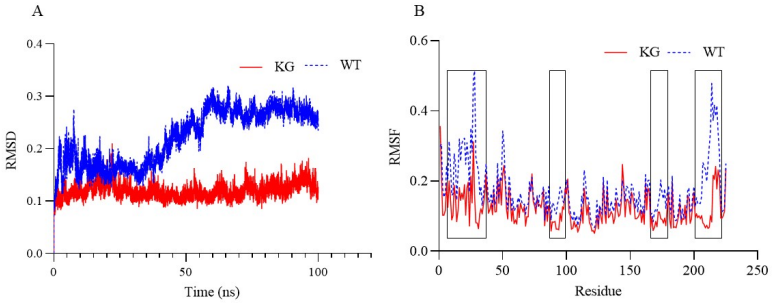


Fig. 1

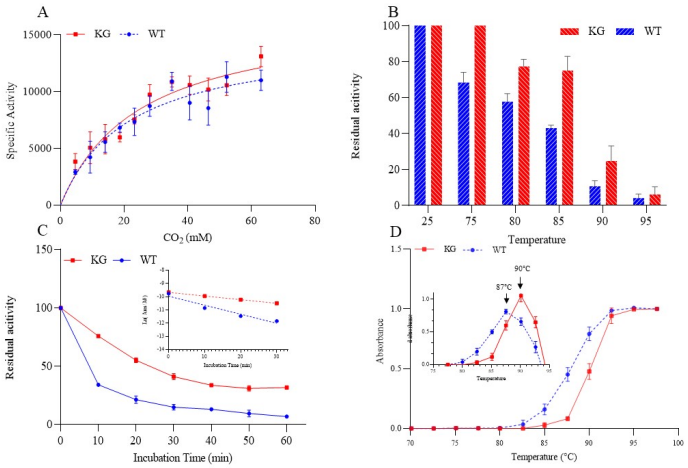
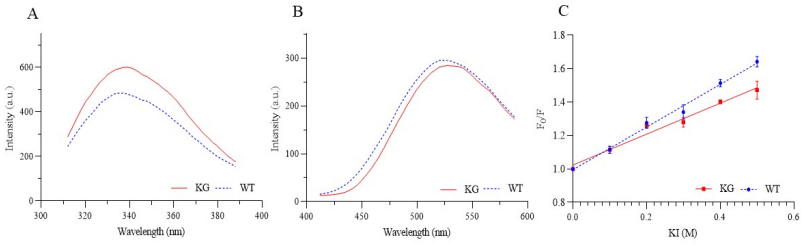


Fig. 2



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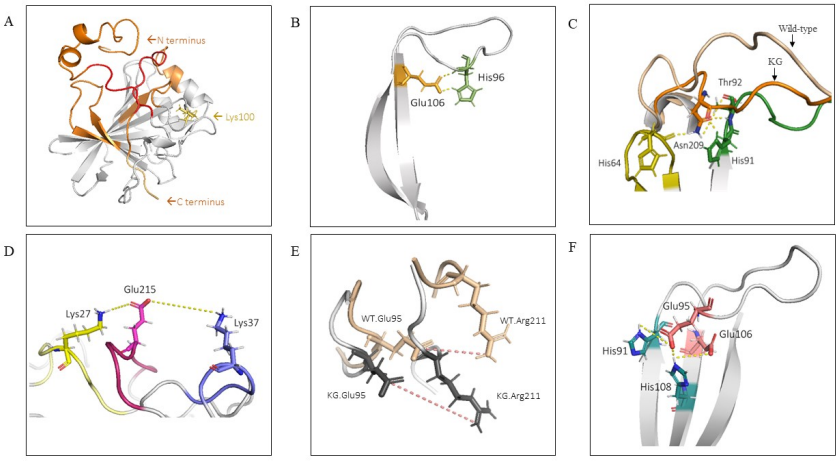

Fig.4

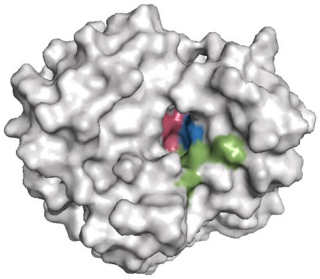

Fig. 5