N°1005 / PC
TOPIC(s) : Synthetic biology, metabolic engineering

Enzymatic Decarboxylation Facilitated by Local-Oriented Electric Field

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PURPOSE OF THE ABSTRACT

Decarboxylation of the aromatic carboxylic acids is an important but challenging reaction in the biocatalytic synthesis of many valuable compounds and has thus attracted great attentions. Enzymatic decarboxylation reaction usually requires cofactor and metal ion for the activity. For example, the decarboxylation of 3,4-dihydroxybenzoic acid by the decarboxylase AroY requires the prenylated flavin mononucleotide (prFMN) as the cofactor[1] and ortho-benzoic acids decarboxylases from the amidohydrolase superfamily needs Mn2+/Mg2+ for the activities[2]. However, the recently characterized gallic acid decarboxylase (AGDC1) is capable of catalyzing the cofactor- and metal-independent non-oxidative decarboxylation of 3,4,5-trihydroxybenzoic acid and 3,4-dihydroxybenzoic acid.[3] In the present study, by using quantum chemical cluster approach, the detailed reaction mechanism of AGDC1 is revealed. Interestingly, it is demonstrated that the build-in local electric field (LEF) in the enzyme is important for the reaction activity. Two lysine residues adjacent to the binding pocket are proven to be the key residues in inducing the LEF. The strengths of the LEFs in AGDC1 and AroY are calculated and compared. It is shown that the LEF in AGDC1 is much stronger than that in AroY. Our findings provide deep insights into the cofactor- and metal-independent enzymatic decarboxylation reaction, and the obtained information are helpful in the mechanism-guided protein engineering of the enzymes.

FIGURES

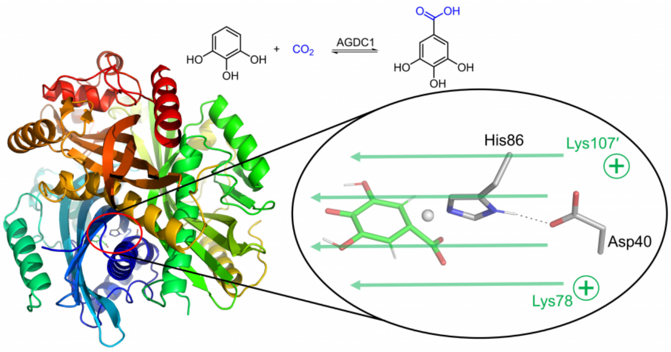

FIGURE 1

The cofactor- and metal-independent decarboxylation reaction of gallic acid decarboxylase facilitated by local-oriented electric field.

Figure 1

FIGURE 2

KEYWORDS

decarboxylase | reaction mechanism | local electric field | density functional theory

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BIBLIOGRAPHY

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