

The active site and substrate binding mode of 1-aminocyclopropane-1-carboxylate oxidase of apple (*Malus domestica* Borkh. cv. Golden delicious) fruit determined by site-directed mutagenesis and comparative modeling studies

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Active sites and substrate bindings of 1-aminocyclopropane-1-carboxylate oxidase (MD-ACO1) catalyzing the oxidative conversion of ACC to ethylene have been determined based on site-directed mutagenesis and comparative modeling methods. Molecular modeling based on the crystal structure of Isopenicillin N synthase (IPNS) provided MD-ACO1 structure. MD-ACO1 protein folds into a compact jelly roll shape, consisting of 9 α -helices, 10 β -strands and several long loops. The MD-ACO1/ACC/Fe(II)/Ascorbate complex conformation was determined from automated docking program, AUTODOCK. The MD-ACO1/FeII complex model was consistent with well known binding motif information (HIS177-ASP179-HIS234). The cosubstrate, ascorbate is placed between iron binding pocket and Arg244 of MD-ACO1 enzyme, supporting the critical role of Arg244 for generating reaction product. These findings are strongly supported by previous biochemical data as well as site-directed mutagenesis data.