

The relationship between substrate specificity of CIP and docking energy

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CIP (*Coprinus cinereus* peroxidase) is fungi peroxidase which catalyzes phenol compounds. It can catalyze the polymerization of ortho-, meta-, and para- phenol compounds. The phenol compounds are phenol, cresol, ethyl phenol, isopropyl phenol, and tert-butyl phenol. All meta- and para- phenol compounds are catalyzed by CIP but o-isopropyl phenol and o-tert-butyl phenol are not catalyzed by CIP. In this presentation, docking energy and distance between Fe atom in heme group and oxygen atom in phenol compounds were calculated. And the relationships between Mn (number-average molecular weight), yield, docking energy and distance were investigated. There is a linear relationship between distance and yield.