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A Chemical Model of Catechol-O-methyltransferase. Methylation of 3,4-Dihydroxybenzaldehyde in Methanol Solution*

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Catechol-O-methyltransferase (COMT, EC 2.1.1.6) catalyzes catecholamine metabolism. It requires Mg^{2+} for the full activity.

The reaction of 3,4-dihydroxybenzaldehyde (LH₂) and dimethyl sulfate (DMS) in forming *m*- and *p*-O-methylated products (vanillin and isovanillin, respectively) in a methanol buffer solution was studied kinetically as a chemical model of this enzyme. The O-methylations, especially *m*-O-methylations, were catalyzed by divalent metal ions such as Cu (II), Mg (II) and Zn (II). A clear Mg (II) catalysis was observed for the first time in this medium. As Mg (II) is an important metal in the COMT catalyzed reaction *in vivo*, this observation is very interesting. Kinetic analyses of the present data and recalculation of a part of the previous data offered the following evidence. In Cu (II) catalysis, a 1:2 complex (CuL₂) was more active than the 1:1 complex (CuL). On the other hand, in Mg (II) catalysis and Zn (II) catalysis, ML was more active than ML₂. These facts show that ML₂ is not always more active than ML, contrary to previous reports. Methanolysis of DMS, a significant side reaction of this model reaction, and dissociation of LH₂ were studied thoroughly as bases for these kinetic analyses.

^{*} 本報告は Chem. Pharm. Bull., 41, 1007—1011(1993)に発表