| | |
|---|---|
| Title | A chemical model of catechol-O-methyltransferase. methylation of 3, 4-dihydroxybenzaldehyde in aqueous solution |
| Sub Title | |
| Author | 菅田, 節朗(Sugata, Setsuro)<br>石原, 静子(Ishihara, Shizuko)<br>渡辺(玉野), 裕子(Watanabe(Tamano), Yuko)<br>永田, 佳子(Nagata, Yoshiko)<br>松島, 美一(Matsushima, Yoshikazu) |
| Publisher | 共立薬科大学 |
| Publication year | 1989 |
| Jtitle | 共立薬科大学研究年報 (The annual report of the Kyoritsu College of Pharmacy). No.34 (1989. ) ,p.75- 75 |
| JaLC DOI | |
| Abstract | |
| Notes | 抄録 |
| Genre | Technical Report |
| URL | https://koara.lib.keio.ac.jp/xoonips/modules/xoonips/detail.php?koara_id=AN00062898-00000034-0075 |

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

Setsuro SUGATA, Shizuko ISHIHARA, Yuko WATANABE (TAMANO), Yoshiko NAGATA and Yoshikazu MATSUSHITA

菅田節朗，石原静子，渡辺(玉野)裕子，永田佳子，松島美一

Catechol-*O*-methyltransferase (COMT, EC 2.1.1.6) catalyzes the transfer of the methyl group of *S*-adenosyl-L-methionine (SAM) to the phenolic group of catechol or substituted catechols. It requires divalent metal ions such as $Mg^{2+}$ for the catalysis. The *O*-methylation *in vivo* occurs almost exclusively on the *m*-hydroxyl group of the catechols, but *in vitro* it occurs at one of the *m*- or *p*-hydroxyl groups.

To elucidate the role of metal ions in *O*-methylation of catechols, the reaction of 3,4-dihydroxybenzaldehyde ($LH_2$) and dimethylsulfate (DMS) to form the *m*- and *p*-*O*-methylated products (vanillin and isovanillin, respectively) was studied. The kinetics of the reaction in aqueous 2-(*N*-morpholino)ethanesulfonate buffer in the presence and the absence of metal ions were measured. The products were determined by means of high-performance liquid chromatography. The *O*-methylation occurred principally at the *p*-hydroxyl group in the absence of divalent metal ions. In the presence of Cu(II), the *m*-methylation was promoted and became predominant. Zn(II) showed a similar but less pronounced effect. The effects were explained in terms of the complex formation of $LH_2$. The second order rate constants for the *m*- and *p*-methylation of the species, $LH_2$, CuL and $CuL_2^{2-}$ by DMS were calculated. The values and their ratio for the *m*-/*p*-reactions increased in the order of $LH_2 < CuL < CuL_2^{2-}$. The reaction may serve as a chemical model for COMT.

* 本報告は *Chem. Pharm. Bull.*, **37**, 1143—1146 (1989) に発表.