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Formation of a Cycotiamine Complex with Fatty Acid in Chloroform*

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The formation of a complex between cycotiamine (CCT), an S-acylated type of thiamine derivative, and a fatty acid (FA) in chloroform has been studied using the solubility method, ^{1}H nuclear magnetic resonance spectroscopy (NMR), and ^{13}C NMR for the purpose of revealing the moieties of CCT needed for an interaction with FA. The apparent stability constants for an equimolar complex between CCT and myristic acid and for CCT and stearic acid were determined (22.9 M^{-1} and 21.7 M^{-1}, at 298 K respectively). A similarity of the pattern of interaction in chloroform to that in 1,2-dichloroethane has been suggested. In the presence of FA, ^{13}C resonance of the carbons adjacent to N-1 in the pyrimidine of CCT were largely shifted upfield. In the presence of FA, the amino proton signal in the pyrimidine of CCT was largely shifted downfield. These results show the necessity of the N-1 nitrogen and the amino group in the pyrimidine of CCT for the interaction. In the presence of CCT, the carboxyl carbon resonance of FA shifted upfleld. This can be understood to result from the destruction of a dimer of FA by the formation of the complex with CCT.

* 本報告は *Chem. Pharm. Bull.*, 38, (11), 2907—2910 (1990) に発表.