

J. Med. Chem., 25 (3), 315–320 (1982)

Quantitative Structure-Inhibitory Activity Relationships of Phenols and Fatty Acids for *Bacillus subtilis* Spore Germination

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ABSTRACT

Phenols and fatty acids were found to inhibit L-alanine-initiated germination of *Bacillus subtilis* spores without altering their heat resistance. Inhibitory effect was defined as the concentration necessary to cause 50% inhibition of the germination rate. The quantitative structure-inhibitory activity relationships for 39 phenols and 7 fatty acids were analyzed. The pH dependency of inhibition showed that the nonionized form of the molecules was responsible for inhibition. Hydrophobicity, which was expressed by the partition coefficient or the distribution coefficient of the compounds, was important for inhibition. In addition to hydrophobicity, the electronic effect, which was expressed by the dissociation constant, played a partial role in phenols. The correlation equation of the fatty acids was similar to those of the alcohols and other hydrophobic compounds, which had been reported earlier. That of the phenols, however, appeared to be different, indicating a different and more complex mechanism of inhibition. The type of inhibition by both compounds was mixed rather than competitive or noncompetitive.

枯草菌芽胞の発芽に対するフェノール類および脂肪酸類の定量的構造 発芽阻止活性相関

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抄録 L-アラニンにより誘起される枯草菌芽胞の発芽が菌の熱耐性に変化を与えることなくフェノール類, 脂肪酸類によって阻害されることを見出した。そこで発芽速度を50%阻害するのに必要な阻害剤濃度を発芽阻止活性と定義し, フェノール類(39種), 脂肪酸類(7種)について, その化学構造と阻止活性の間の相関を定量的に解析した。発芽阻止に対するpH依存性の検討により, 阻害剤の非解離分子種が阻害に関与することが判明した。また, この阻害作用において, 分子の疎水性(油中分配係数をパラメータとする)が重要な因子であった。さらにフェノールでは, 疎水性に加え静電的効果(酸解離定数をパラメータとする)も寄与することが認められた。脂肪酸による阻害式は, 先に報告したアルコール類, 種々の疎水性化合物に対して得られたものと類似した。一方, フェノール類についての相関式は異なっており, より複雑な阻害機構の存在が示唆された。