

论文

芳环上96种常用取代基的Q型聚类分析法

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摘要:

本文对芳环上96种常用取代基采用L(A)、n、F、R、σ_m和σ_p六种化学结构参数,以相似系数Cosθ_{jk}作为分类统计量,对取代基进行Q型标准化聚类分析。根据实际需要分成5群、10群及18群。可供药物研究者选择合成对象作参考。本文采用自编ALGOL-60语言程序在国产709机上完成全部计算。

关键词: 聚类分析 药物设计 先导化合物

Q-MODEL CLUSTER ANALYSIS OF 96 COMMON AROMATIC SUBSTITUENTS

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Abstract:

In drug design, the large number of possible substituents that might be selected for an initial set of derivatives presents a formidable problem in decision making. By factoring such a set into more or less homogeneous subgroups with respect to various chemical structural parameters of importance, one can focus upon such special considerations as hydrophobic effects, metabolic behavior, or ease of synthesis. If the clusters are formed by an objective procedure such as resemblance coefficient between the points in a parameter space, selecting one derivative from each cluster will tend to give a maximum range in parameter type and help to establish a viable structure-activity relationship more rapidly. In this paper, 96 common aromatic substituents have been clustered into 5, 10, and 18 clusters with respect to various combinations of length L (A) in Sterimol system, the lipophilie n constant, electronic Swain and Luptontype F and R constants, σ_m and σ_p constants. The dendrogram of classification is also provided. These clusters may be applied to selecting molecules in drug design.

Keywords: Drug design Lead compound Cluster analysis

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2. 杨丰庆;李绍平;陈莹;刘倩青;王一涛;董婷霞;詹华强.中药莪术GC-MS指纹图谱研究[J]. 药学学报, 2005,40(11): 1013-1018

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