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研究论文

手性分子与手性拓扑指数

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摘要 应用自制的有机化合物结构解析专家系统ESESOC, 对与28个外消旋类化合物(特殊的氨基酸)分子手性中心有关的对称性问题进行了判别, 如对称面、对称点和对称轴等. 同时用的开发的程序对这些化合物的构型进行了自动识别和标示. 在此基础上, 以手性拓扑指数为参数, 利用Fisher意义下的分析和人工神经网络法, 对这些化合物的对映体进行了高效液相色谱分离中先后淋洗出的的对映体进行分类判别. 结果表明, 人工神经网络法优于Fisher意义下的判别分析.

关键词 手性分子 手性拓扑指数 构型 手性中心 Fisher意义下的分析 人工神经网络法

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Chirality Molecules and Chiral Topological Indices

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Abstract In this paper, the symmetry of 28 racemoids(unusual amino acids), such as symmetrical face, symmetrical node and axis, were recognized by using expert system of structure elucidation of organic compound, and the configurations of those compounds were recognized by using the program developed by our laboratory. On the basis, with chiral topological indices, the elution order with HPLC were performed by using Fisher analysis and artificial neural network for enantiomers of these compounds. Artificial neural network gave out a better result than that obtained by using Fisher analysis.

Key words Chiral molecule Chiral topological indice Configuration Chiral center Fisher analysis Artificial neural network

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