研究论文

后叶催产素的定量构效关系研究

梅虎[1,2], 杨力[1,2], 舒茂[1,2], 刘丽[2], 李志良[1,3]

1. 重庆大学生物医学工程重庆市重点实验室,
2. 生物工程学院,
3. 化学化工学院, 重庆　400044

摘要　　基于氨基酸物化性质的描述子矢量VHSE, 对21个后叶催产素类似物进行结构表征. 经逐步回归与偏最小二乘相结合的变量筛选技术, 根据模型的外部预测结果, 筛选得到一个最优的9变量组合. 应用该变量组合对21个后叶催产素类似物的促宫缩活性进行偏最小二乘建模, 模型复相关系数R^2为92.6%, 留一法和留组法交互验证Q^2分别为78.3%和79.4%. 结果表明, 后叶催产素的促宫缩活性主要与第3号氨基酸残基的疏水性、立体结构和电性性质以及第8号氨基酸残基的电性特征密切相关.

关键词　　As a new set of amino acid descriptors, VHSE(principle component score vector of hydrophilicity, steric, and electronic variables) scales were applied to QSAR studies on 21 oxytocin analogues. Firstly, stepwise multiple regression combined with partial least squares was used to screen variables. According to the result of external validation, an optimal variable subset with 9 variables was obtained. Then, this optimal variable subset was employed to establish PLS model on all 21 samples with the results of the squared multiple correlation coefficient (R^2), leave-one-out cross-validation R^2, and n-fold cross-validation(n=5) R^2 were 92.6%, 78.3%, and 79.4%, respectively. The results show that oxytocic activity was closely related to the hydrophobic, steric, and electronic properties in positions 3 and electronic property in position 8 of oxytocin analogues.

分类号　0641

Quantitative Structure-activity Relationships Studies on Oxytocin Analogues

MEI Hu[1,2], YANG Li[1,2], SHU Mao[1,2], LIU Li[2], LI Zhi-Liang[1,3]*

1. Key Laboratory of Biomedical Engineering of Chongqing,
2. College of Biological Engineering,
3. College of Chemistry and Chemical Engineering, Chongqing University, Chongqing 400044, China

Abstract　VHSE; 后叶催产素; 肽; 定量构效关系; 偏最小二乘

Key words　VHSE　Oxytocin　Peptide　Quantitative structure-activity relationships　Partial least squares

通讯作者 李志良 zlli2662@163.com