高等学校化学学报 2009, 30(10) 1960-1964 DOI: ISSN: 0251-0790 CN: 22-1131/O6

论文

纤维堆囊菌发酵液中埃博霉素含量的HPLC法分析

孟凡欣, 郭伟良, 逯家辉, 杜林娜, 李又欣, 滕利荣

吉林大学生命科学学院, 长春 130012

摘要:

采用反馈神经网络结合遗传算法(BPANN-GA)对高效液相色谱(HPLC)法同时测定纤维堆囊菌(*Sorangium cellulosum*)代谢物中埃博霉素A(Epo A)和埃博霉素B(Epo B)含量的条件进行优化, 采用均匀设计(U_{12}^{3})方案对流动相中乙腈的体积分数、色谱柱温度和流动相的pH等3个因素进行实验设计; 以色谱函数(COF)值为优化指标, 运用双层反馈神经网络建立色谱优化函数(COF)值, 考察因素间的预测模型, 采用Levenberg-Marquardt backpropagation算法对所建立的神经网络预测模型进行训练, 以逼近度(D_a)为优化参数, 选择预测模型的最适隐含层节点数. 最优预测模型预测的COF值与实验值之间的相关系数(R)达到0.98165, 采用遗传算法在实验考察范围内进行全局寻优, 得到最优化的HPLC分析条件: 流动相中乙腈体积分数为29.2%, 色谱柱温度为34 ℃, 流动相pH为4.23. 在此最优条件下对纤维堆囊菌代谢产物进行HPLC分析, 结果表明, 该方法对两种埃博霉素色谱峰均具有较好的分离度.

关键词: 反馈神经网络(BPANN); 遗传算法(GA); 埃博霉素; 高效液相色谱(HPLC)

HPLC Optimization for Analysis of Epothilones in *Polyangium Cellulosum* Fermentation Metabolites

MENG Fan-Xin, GUO Wei-Liang, LU Jia-Hui, DU Lin-Na, LI You-Xin, TENG Li-Rong*

College of Life Science, Jilin University, Changchun 130012, China

Abstract:

Back-propagation artificial neural network combined with genetic algorithm(BPANN-GA) was applied to optimize the high performance liquid chromatography(HPLC) conditions for the determination of epothilone A(Epo A) and epotholine B(Epo B) simultaneously in *Polyangium cellulosun* metabolites. The concentration of acetonitrile in mobile phase, column temperature and the pH of mobile phase were selected as casual factors and a three-factor-twelve-level uniform design(U_{12}^{3}) was used for experiment design. A two-layer back-propagation artificial neutral network(BPANN) was applied to model for the correlation between the casual factors and chromatography optimization function(COF) values, which was chosen as the criterion. Levenberg-Marquardt algorithm was used for training the BPANN. The BPANN model was optimized by selecting the most suitable numbers of hidden neurons depending on the degree of approximation(D_a). The correlation coefficient(R) between the COF values obtained by BPANN model and the experiment values was 0.98165. While the optimum BPANN model was developed, genetic algorithm(GA) was applied to find out global dissolution in modeling range. The optimum HPLC conditions obtained by BPANN-GA were as follows: the concentration of acetonitrile in mobile phase was 29.2%(volume fraction); the column temperature was 34 ℃ and pH of mobile phase was 4.23. The validation experiment at the optimum conditions was performed, and the satisfied chromatogram was obtained.

Keywords: Back-propagation artificial neural network(BPANN); Genetic algorithm(GA); Epothilone; High performance liquid chromatography(HPLC)

收稿日期 2009-01-24 修回日期 网络版发布日期

DOI:

基金项目:

中国医学基金会新药发展基金(批准号: 20061108)资助.

通讯作者: 滕利荣, 男, 教授, 博士生导师, 主要从事微生物与生化药学研究. E-mail: tenglr543@gmail.com

作者简介:

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