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过程系统工程

香茶菜属植物二萜化合物核磁共振碳谱模拟

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摘要 将原子电性作用矢量(AEIV)和原子杂化状态指数(AHSI)应用于香茶菜属植物二萜化合物核磁共振碳谱(13C NMR)模拟。分别利用多元线性回归(MLR)和人工神经网络(CNN)建立定量结构波谱相关(QSSR)模型，同时采用内部及外部双重验证的办法对所得模型稳定性能进行了深入分析和检验。建模计算值、留一法(LOO)交互校验(CV)预测值和外部样本预测值的复相关系数分别为Rcum=0.9724, QLOO=0.9723, Qext=0.9738(MLR)； Rcum=0.9957, Qext=0.9956(CNN)。结果表明：AEIV，AHSI与13C NMR谱化学位移显著相关，且CNN所建模型明显优于MLR。

关键词 香茶菜属植物二萜化合物 定量结构波谱相关 13C NMR化学位移 原子电性作用矢量 原子杂化状态指数

分类号

Spectroscopic simulation of 13C nuclear magnetic resonance of diterpenoids of isodon species

Abstract

Atomic electronegativity interaction vector (AEIV) and atomic hybridization state index (AHSI) were used for establishing the quantitative structure-spectroscopy relationship (QSSR) model of 13C NMR chemical shifts of isodon diterpenoid compounds. Multiple linear regression (MLR) and computational neural network (CNN) were used to create the models, and the estimation stability and generalization ability of the models were strictly analyzed by both internal and external validations. The established MLR and CNN models were correlated with experimental values and the correlation coefficients of model estimation, leave-one-out (LOO) cross-validation (CV), and predicted values of external samples were R cum=0.9724, R CV=0.9723, Q ext=0.9738(MLR); R cum=0.9957, Q ext=0.9956(CNN), respectively. The results indicated that CNN gave significantly better prediction of 13C NMR chemical shifts for isodon diterpenoids than MLR. Satisfactory results showed that AEIV and AHSI were obviously good for modeling 13C NMR chemical shifts of isodon diterpenoid compounds.

Key words diterpenoids of isodon species quantitative structure-spectrum relationship 13C NMR chemical shift atomic electronegativity interaction vector atomic hybridization state index

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