

基于模拟退火波长优化的草莓坚实度近红外光谱检测 Detection of Strawberry Firmness by NIR Wavelength Selection Based on Simulated Annealing Algorithm

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摘要: 为提高近红外光谱技术检测草莓坚实度模型的精度和鲁棒性, 研究了一种基于模拟退火算法的波长优选方法, 并找到一种与该算法配套的光谱预处理方法。利用光谱仪和物性仪分别采集草莓样品近红外漫反射光谱和坚实度数据, 并采用标准正交变换、多元散射校正、一阶导数、二阶导数等方法对原始光谱进行预处理; 最后, 利用模拟退火算法优选与草莓坚实度高度相关的波数点变量, 结合偏最小二乘法建立草莓坚实度预测模型。结果表明: 经过标准正交变换预处理后, 采用模拟退火算法优选出24个波数点, 在主成分数为5时, 建立的偏最小二乘模型具有最佳预测效果, 模型校正集样本相关系数 r_c 为0.9342, 校正均方根误差为0.665 N/cm²; 预测样本相关系数 r_p 为0.9197, 预测均方根误差为0.673 N/cm²。研究表明: 模拟退火算法可以提高近红外模型预测草莓坚实度的精度和鲁棒性, 并降低预测模型复杂度。 In order to improve the accuracy and robust of NIR spectroscopy modules in predicting the firmness of strawberry, simulated annealing algorithm (SAA) was used to select the wavenumbers in NIR spectra. A preprocessing method was also selected to adapt the SAA. Firstly, 150 strawberries were selected to collect NIR spectra. Secondly, preprocessing methods, such as SNV, MSC, 1st order derivation, 2nd order derivation, were used to denoise the NIR spectra of strawberry. Thirdly, 24 wavenumbers were selected by simulated annealing algorithm. At last, partial least square was employed to establish the calibration models of firmness. The calibration model was obtained with the correlation coefficient r_c of 0.9342, the root mean square error of calibration of 0.665 N/cm² and the correlation coefficient r_p of 0.9197, the root mean square error of prediction of 0.673 N/cm². The results show that SAA can improve the robust and accuracy and simplify NIR spectra models.

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