

[本期目录](#) | [下期目录](#) | [过刊浏览](#) | [高级检索](#)[\[打印本页\]](#) [\[关闭\]](#)**论文****近红外光谱与组合的间隔偏最小二乘法测定清开灵四混液中总氮和栀子苷的含量**朱向荣^{1,2}, 李娜², 史新元², 乔延江², 张卓勇¹

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摘要:

应用近红外光谱分析技术结合化学计量学方法, 建立了中药清开灵注射液中间体总氮和栀子苷含量测定的新方法。首先采用Kernard-Stone法对训练集样本和预测集样品进行分类, 然后应用组合的间隔偏最小二乘法(Synergy interval partial least squares, siPLS)对所得近红外透射光谱进行有效谱段范围的选择以及二者定量校正模型的建立, 并对光谱预处理方法进行了详细的讨论。所建立的总氮和栀子苷校正模型的预测相关系数(R)分别为0.999和0.708; 交叉验证误差均方根(RMSECV)均为0.023; 预测误差均方根(RMSEP)分别为0.074和0.159; 预测结果表明, 本实验所建方法快速、无损且可靠, 可推广并应用于中药注射液中间体的在线质量控制。

关键词: 近红外光谱 清开灵注射液中间体 Kernard-Stone法 组合的间隔偏最小二乘法 在线控制

Analysis of Geniposide and Total Nitrogen Content in Qingkailing Injection Intermediate by Near Infrared Spectroscopy and Synergy Interval Partial Least Squares

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Abstract:

Near infrared spectrometry combined with chemometric methods was used for establishing a new method to determine the content of total nitrogen and geniposide in Qingkailing injections. The training and testing sets are partitioned by Kernard-Stone algorithm. Synergy interval partial least squares (siPLS) is used for selecting effective spectral regions and building the quantitative calibration models of the total nitrogen and geniposide. Pre-treatments of spectra are discussed in detail. Correlation coefficient obtained is 0.999, RMSECV is 0.023, RMSEP is 0.074 for the total nitrogen, and correlation coefficient is 0.708, RMSECV is 0.023, RMSEP is 0.159 for geniposide, respectively. The predictive results show that the proposed method is rapid, non-destructive and credible, which can be applied to control the quality of Chinese medicine injection online in industry scenes extensively.

Keywords: Near infrared spectroscopy Qingkailing injection intermediate Kernard-Stone algorithm method Synergy interval partial least squares(siPLS) Online control

收稿日期 2007-10-25 修回日期 1900-01-01 网络版发布日期

DOI:

基金项目:

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参考文献:

1. Yan Shi-kai, Luo Guo-an, Wang Yi-ming, et al.. Journal of Pharmaceutical and Biomedical Analysis [J], 2006, 40(4): 889—895
2. Zhang Hong-yang, Huo Ping, Luo Guo-an, et al.. Analytica Chimica Acta[J], 2006, 577(8): 190—200
3. Yan Shi-kai, Xin Wen-feng, Luo Guo-an, et al.. Chemical & Pharmaceutical Bulletin[J], 2005, 53 (11): 1392—1395
4. Yan Shi-kai, Xin Wen-feng, Luo Guo-an, et al.. Journal of Chromatography A[J], 2005, 1090: 90—97
5. Zhang Jian, Luo Guo-an. Journal of Chromatography B[J], 2006, 837: 11—17
6. YANG Hai-Lei(杨海雷), LIU Xue-Song(刘雪松), QU Hai-Bin(瞿海斌), et al.. Chinese Traditional and Herbal Drugs(中草药)[J], 2005, 36(6): 912—915
7. GU Xiao-Yu(谷筱玉), XU Ke-Xin(徐可欣), WANG Yan(汪曦). Spectroscopy and Spectral Analysis(光谱学与光谱分析)[J], 2006, 26(9): 1618—1620
8. Chan C. O., Chu C. C., Daniel K. W. M., et al.. Analytica Chimica Acta[J], 2007, 592: 121—131
9. YU Ke(虞科), HU Chu-Chu(胡楚楚), CHENG Yi-Yu(程翼宇). Chinese Pharmaceutical Journal(中国药学杂志)[J], 2006, 41(3): 226—229
10. CHENG Biao(成飙), WU Xiao-Hua(吴晓华), CHEN De-Zhao(陈德钊). Spectroscopy and Spectral Analysis(光谱学与光谱分析)[J], 2006, 26(10): 1923—1927
11. ZHAO Chen(赵琛), QU Hai-Bin(瞿海斌), CHENG Yi-Yu(程翼宇). Spectroscopy and Spectral Analysis(光谱学与光谱分析)[J], 2004, 24(1): 50—53
12. YE Zheng-Liang(叶正良), YU Ke(虞科), CHENG Yi-Yu(程翼宇). Chem. J. Chinese Universities(高等学校化学学报)[J], 2007, 28(3): 441—444
13. Nørgaard L., Saudland A., Wagner J., et al.. Applied Spectroscopy[J], 2000, 54: 413—419
14. Leardi R., Nørgaard L.. Journal of Chemometrics[J], 2004, 18: 486—497
15. Luiz C. M. Pataca, Waldomiro Borges Neto, Maria C. Marcucci, et al.. Talanta[J], 2007, 71: 1926—1931
16. Navea S., Tauler R., Anna de Juan. Analytical Biochemistry[J], 2005, 336: 231—242
17. Zou Xiao-bo, Zhao Jie-wen, Huang Xing-yi, et al.. Chemometrics and Intelligent Laboratory Systems[J], 2007, 87: 43—51
18. Kennard R. W., Stone L. A. S.. Technometrics[J], 1969, 11: 137—148
19. Kocjani R., Zupan J.. Chemometrics and Intelligent Laboratory Systems[J], 2000, 54: 21—34
20. Siano G. G., Goicoechea H. C.. Chemometrics and Intelligent Laboratory Systems[J], 2007, 88: 204—212
21. Chen Da, Cai Wen-sheng, Shao Xue-guang. Chemometrics and Intelligent Laboratory Systems [J], 2007, 87: 312—318
22. LU Wan-Zhen(陆婉珍), YUAN Hong-Fu(袁洪福), XU Guang-Tong(徐广通), et al.. Modern Near Infrared Spectroscopy Analytical Technology(现代近红外光谱分析技术)[M], Beijing: China Petrochemical Press, 2000: 20—26

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2. 叶正良, 虞科, 程翼宇 .一种基于小波变换的近红外化学指纹图谱分析方法[J]. 高等学校化学学报, 2007, 28 (3): 441-444
3. 郭隆海, 袁洪福, 邱藤, 李效玉.苯乙烯/丙烯酸正丁酯乳液聚合反应过程中残余单体含量的实时监测[J]. 高等学校化学学报, 2008, 29(6): 1255-1261
4. 郝勇, 蔡文生, 邵学广.复杂样品近红外光谱定量分析模型的构建方法[J]. 高等学校化学学报, 2009, 30(1): 28-31
5. 张勇, 丛茜, 谢云飞, 赵冰.烟草组分的近红外光谱和支持向量机分析[J]. 高等学校化学学报, 2009, 30(4): 697-700

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