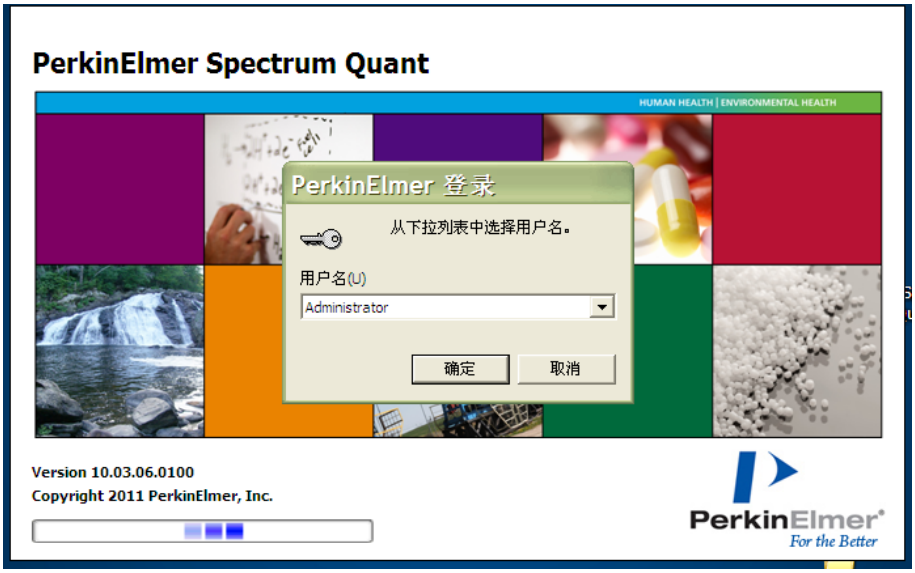
Spectrum Quant Beer’s Law 定量软件操作说明

适用于 Spectrum Quant Version10.03.06 及以上版本

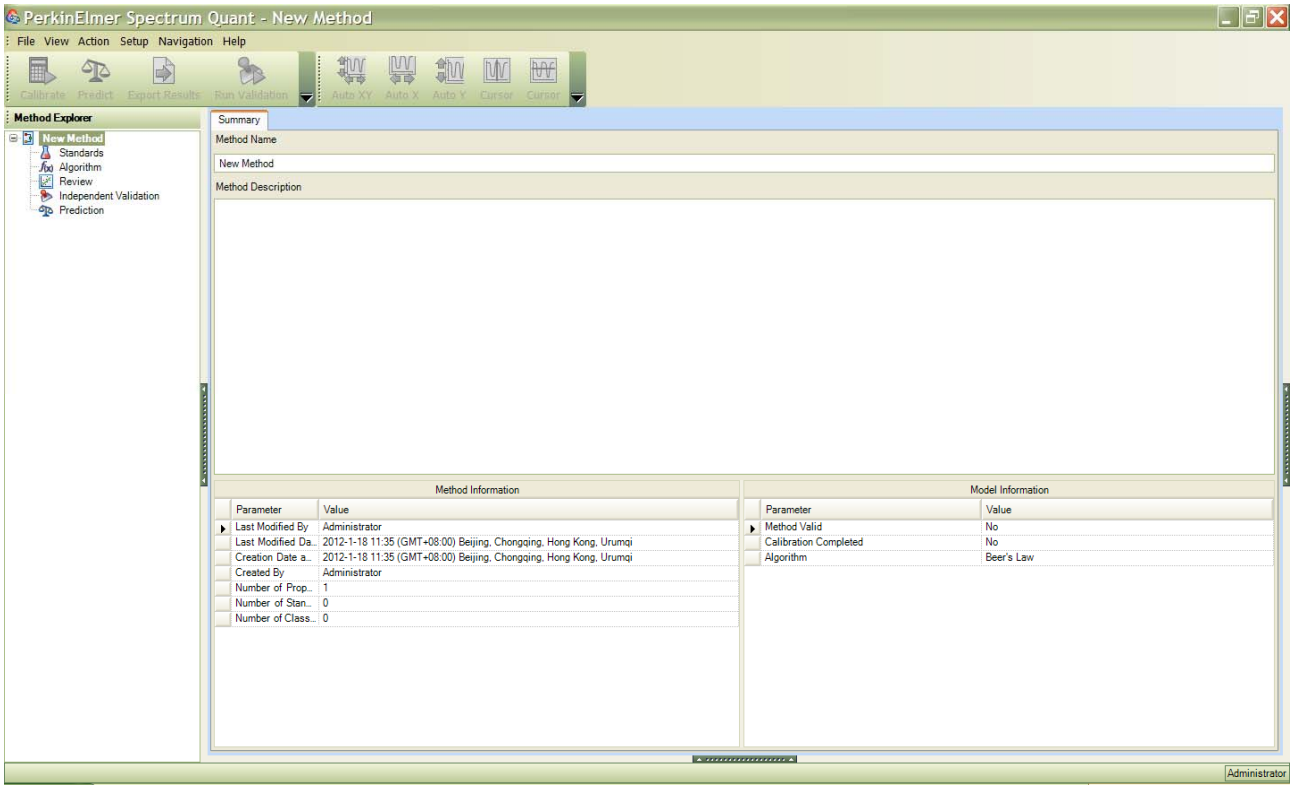
用此软件建立定量方法之前，配置相应浓度梯度的标样，纵坐标以吸光度 A 为单位用 Spectrum 软件控制红外光谱仪依次扫描所有标样的红外吸收光谱图，保存在电脑硬盘指定路径文件夹中备用。

双击桌面 

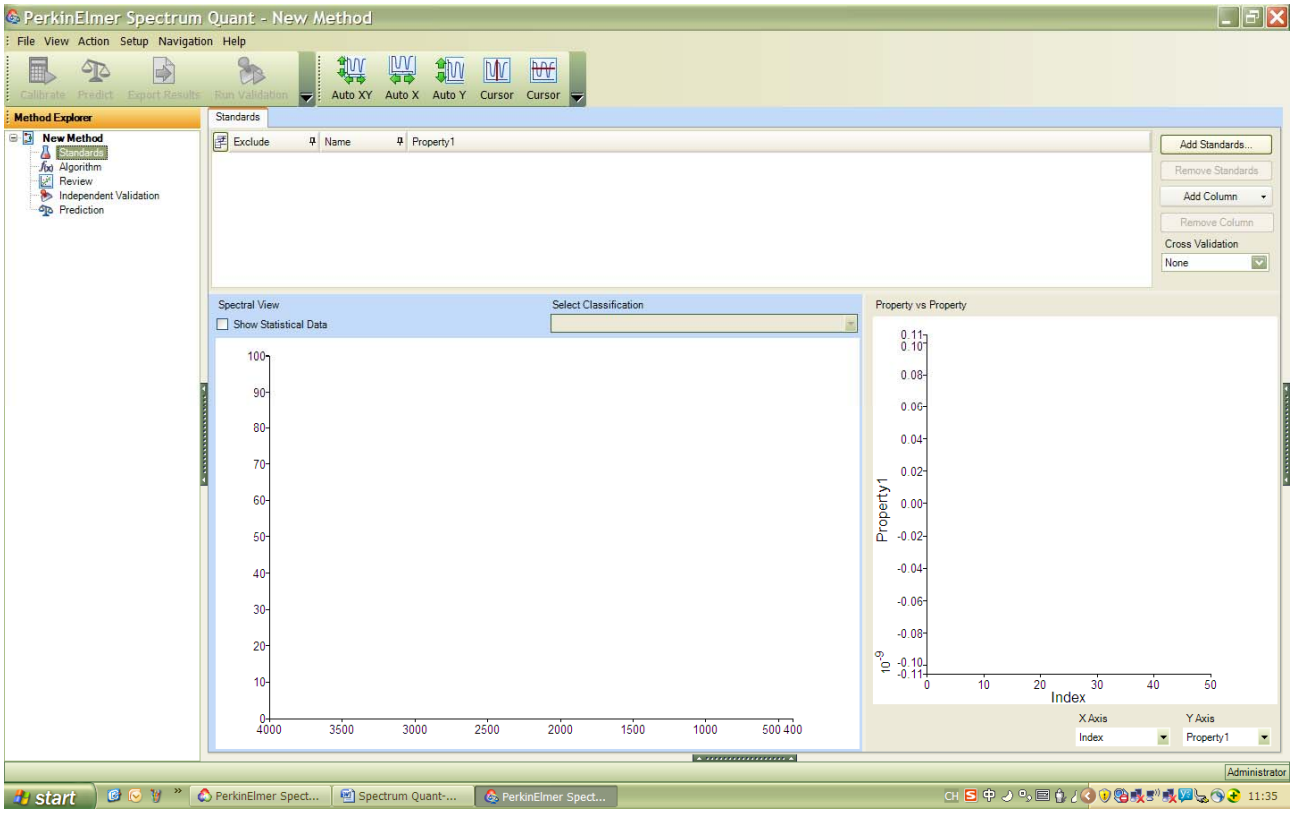
图标打开此软件



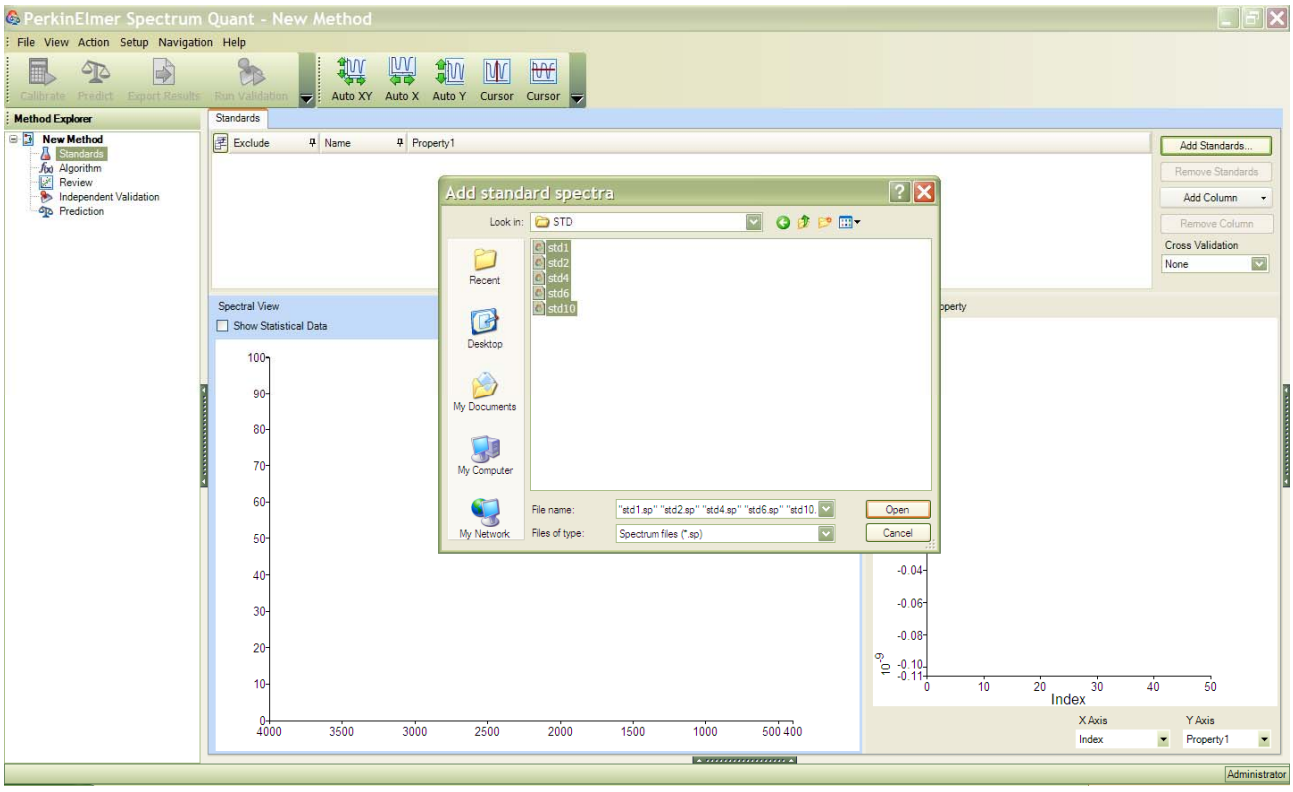
点击<确定>进入软件工作界面



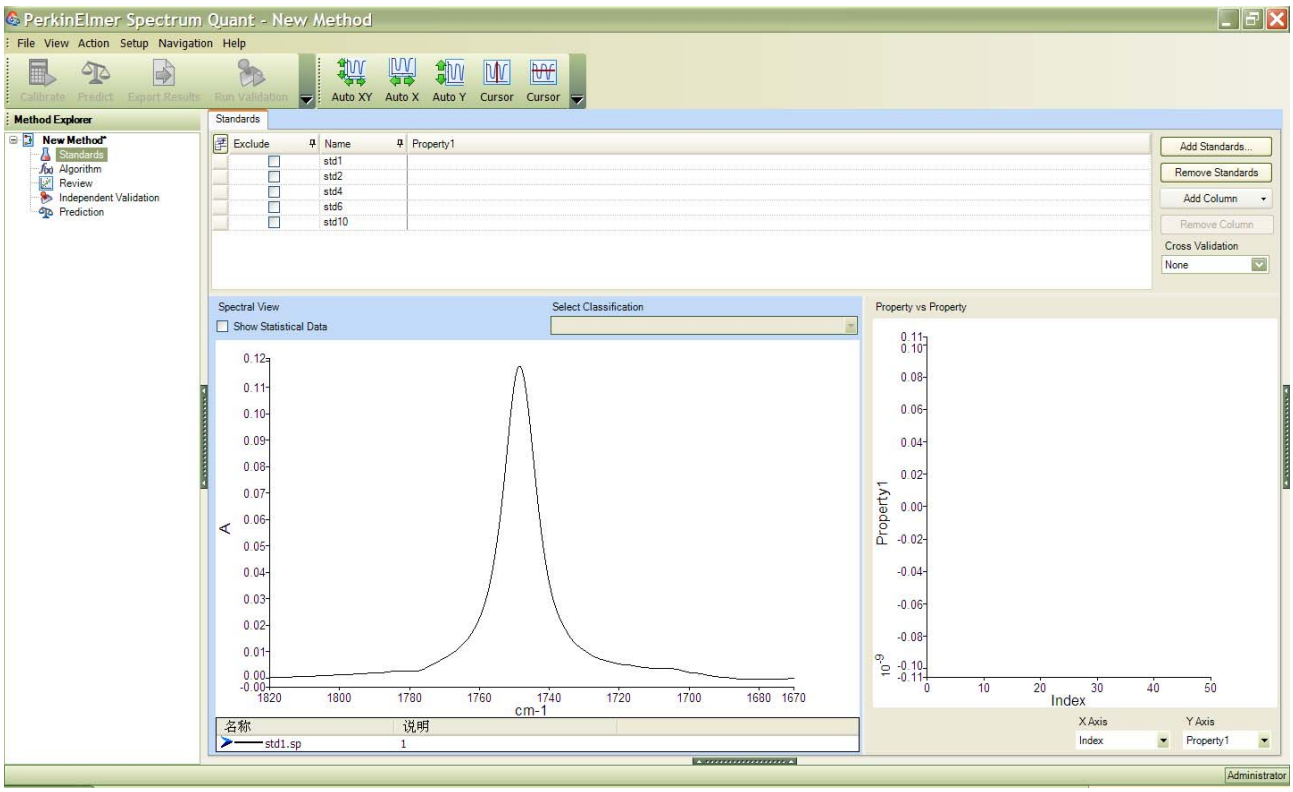
新方法<New Method>栏，输入即将建立的新方法名称<Method Name>，还可以输入方法描述信息<Method Description>，然后点击标样<Standards>栏



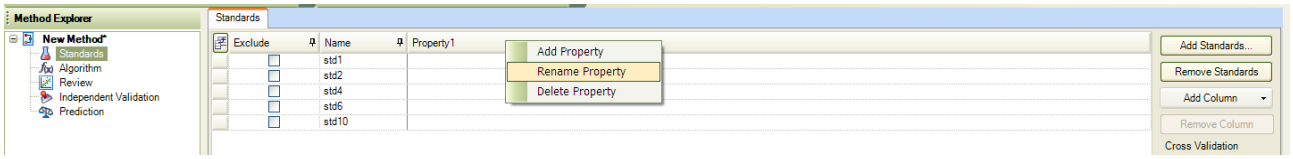
添加标样光谱图　　点击添加标样<Add Standards>，找到相应标样光谱文件(事先已测试好的)存储路径



在事前保存的文件夹中选中标样光谱文件名，点击打开<Open>

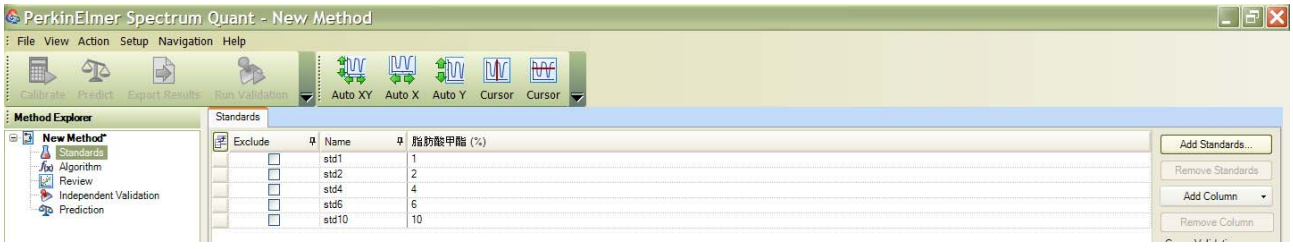


输入组份名称及浓度单位，在组份<Property1>上点击鼠标右键，选择重命名组份<Rename Property>，



输入组份名称<Property name>及单位<Units>，如脂肪酸甲酯，%，点击 OK

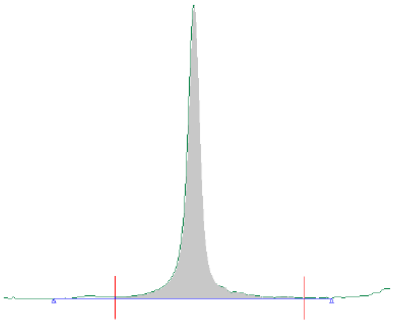
输入每个标样对应的浓度值，在每个标样名后面的框中直接双击鼠标左键即可输入。输完之后点击算法<Algorithm>栏



点击<Beer's Law-脂肪酸甲酯>，选择相应的定量方式<Peak Type>：有积分面积<Area>，峰高(确定波数处)<Height>，最大峰高(某一波数范围内)<Max Height>

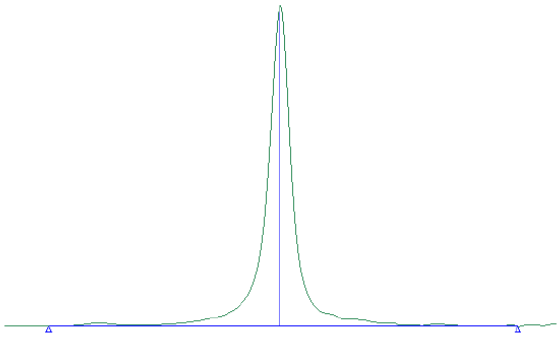
Area

Area is defined by Start and End abscissa values. If no bases are selected, the Area is measured from the curve to zero absorbance. If one or two bases are selected, the Area is measured from the curve to the baseline. For example, the peak Area markers with two base points are shown here:



Height

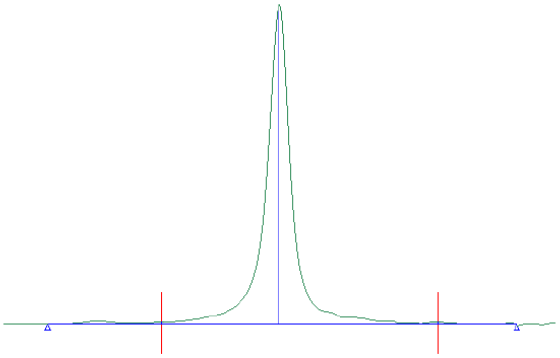
Height is defined by an abscissa value (X in the table). If no bases are selected, the Height is measured from the curve to zero absorbance. If one or two bases are selected, the Height is measured from the curve to the baseline. For example, the Height markers with two base points are shown here:



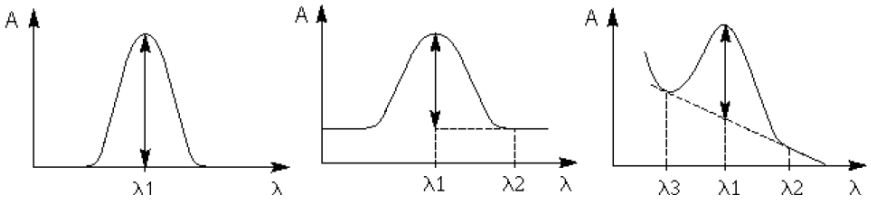
Max Height

Max Height is defined by Start and End abscissa values. The Max Height is the maximum peak height between the start and end abscissa values. If no bases are selected, the Max Height is measured from the curve to zero absorbance. If one or two bases are selected, the Max Height is measured from the curve to the baseline.

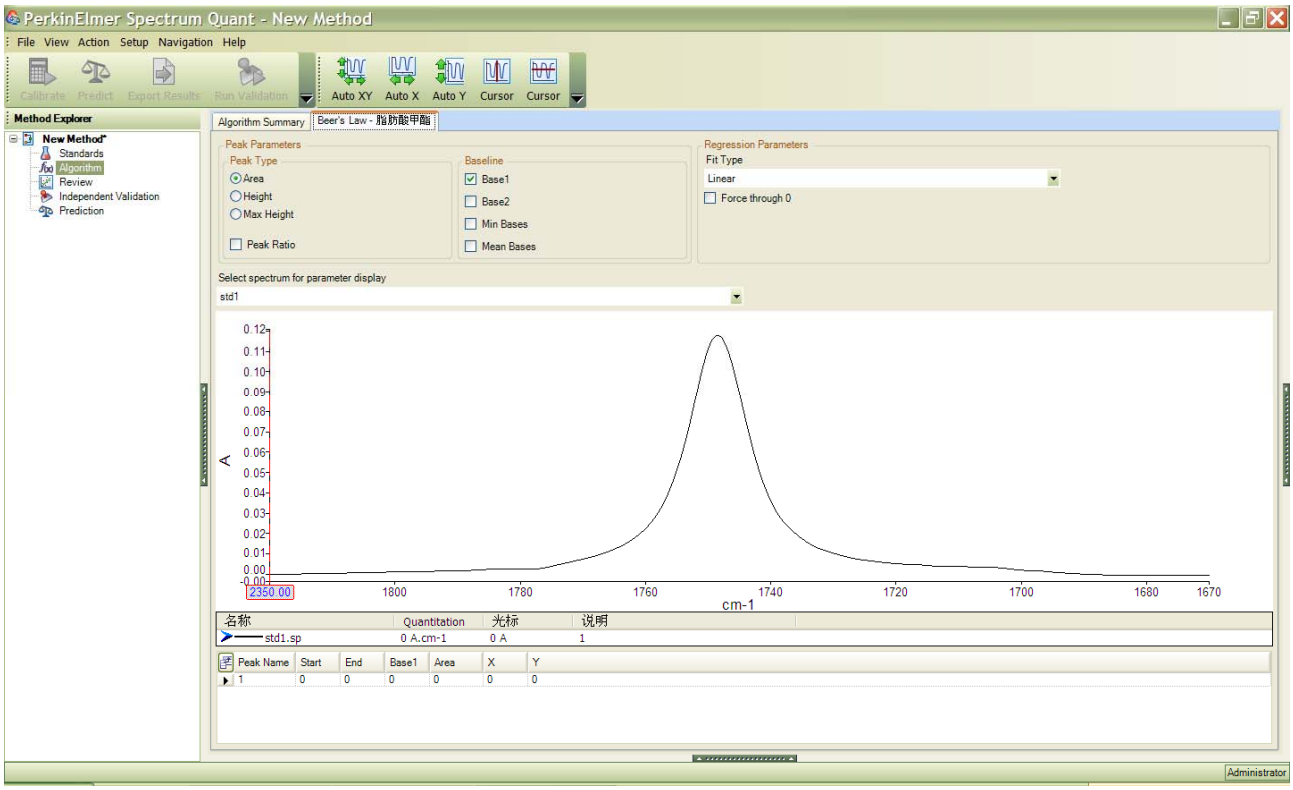
For example, the height markers when Max Height is selected with two base points are shown here:



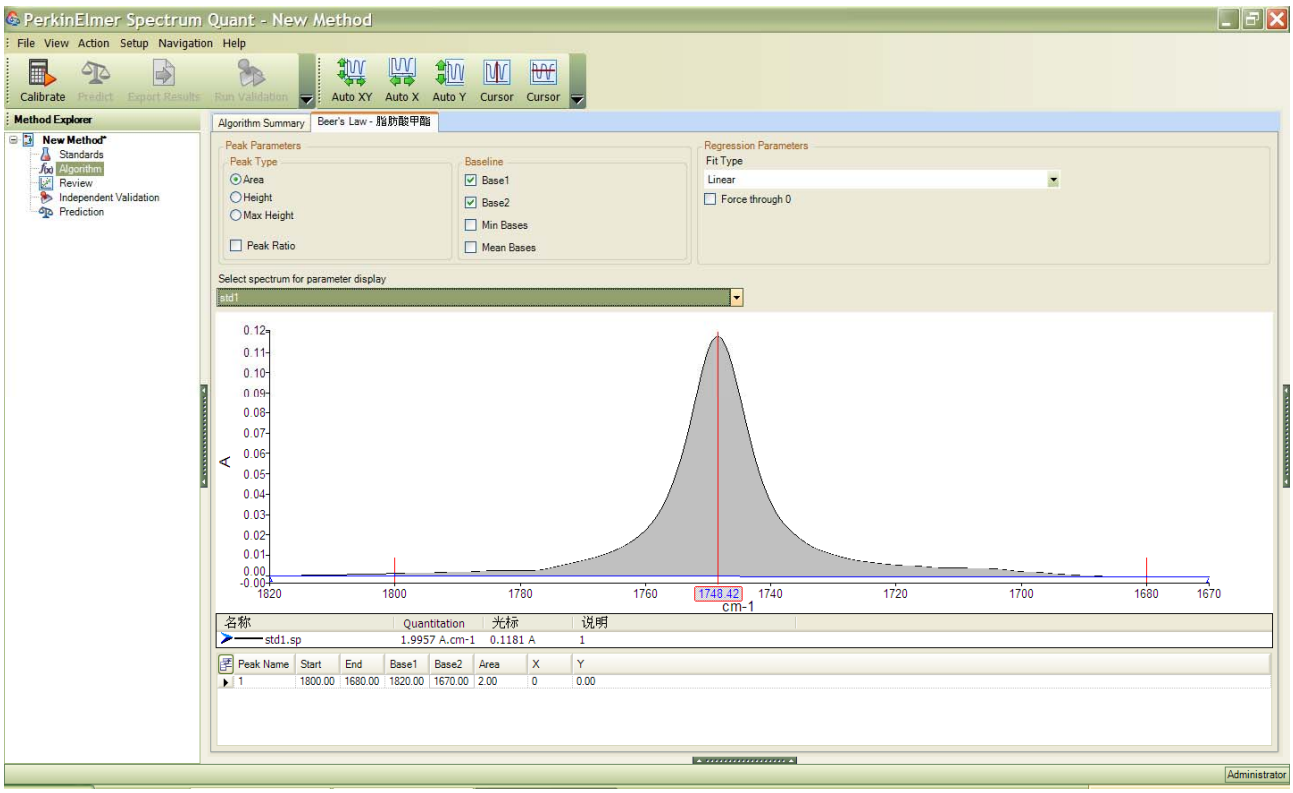
峰比值<Peak Ratio>是指用两个吸收峰的峰面积或峰高或最大峰高的比值，跟浓度做线性回归
选择基线校正模式<Baseline>：有一点基线校正<Base 1>，两点基线校正<Base 1>和<Base 2>
选择不进行基线校正还是单点基线校正或两点基线校正，取决于基线的形状，



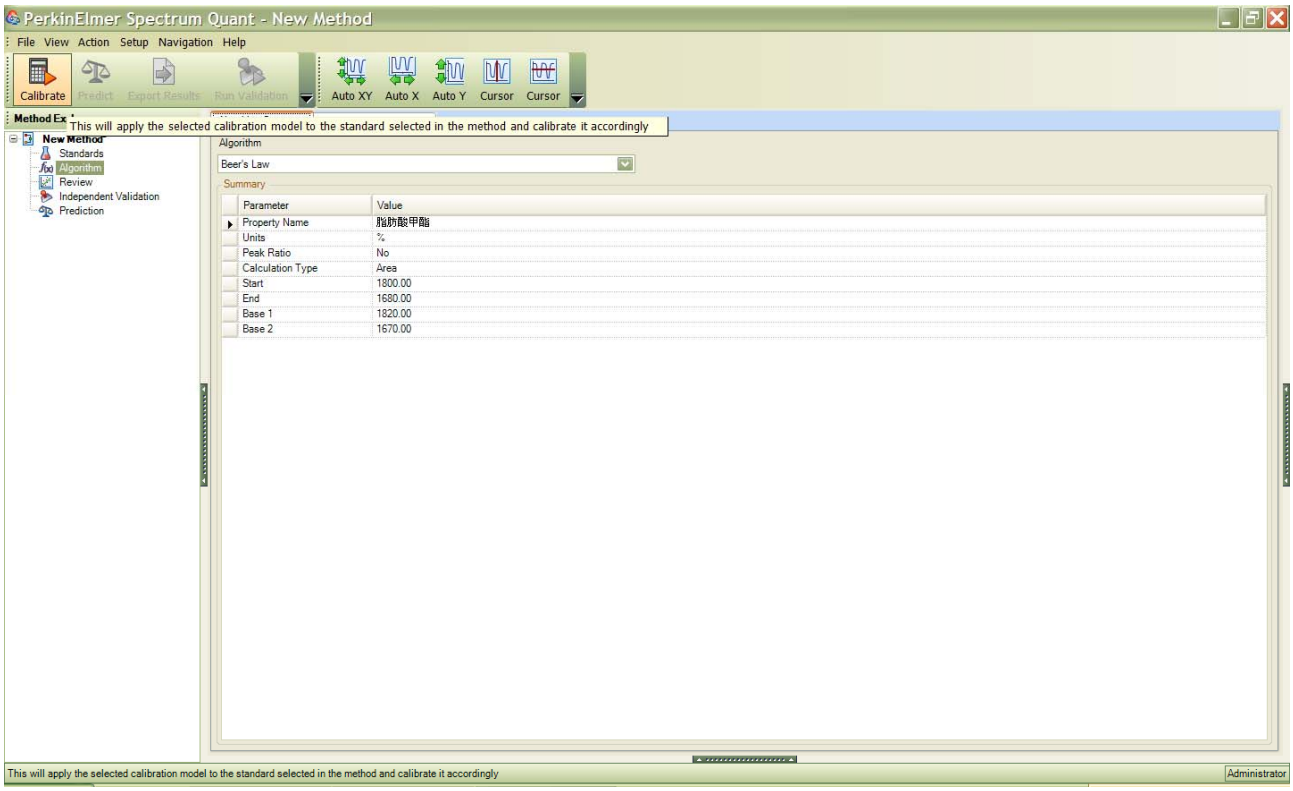
如上图的三种吸收曲线，就应该分别选用不进行基线校正，单点基线校正和两点基线校正
回归方式<Fit Type>默认为线性回归<Linear>；Force Through 0 指是否强制过零点



输入峰面积或峰高或最大峰高计算的起始波数范围<Start><End>，输入基线点的波数位置<Base 1><Base 2>

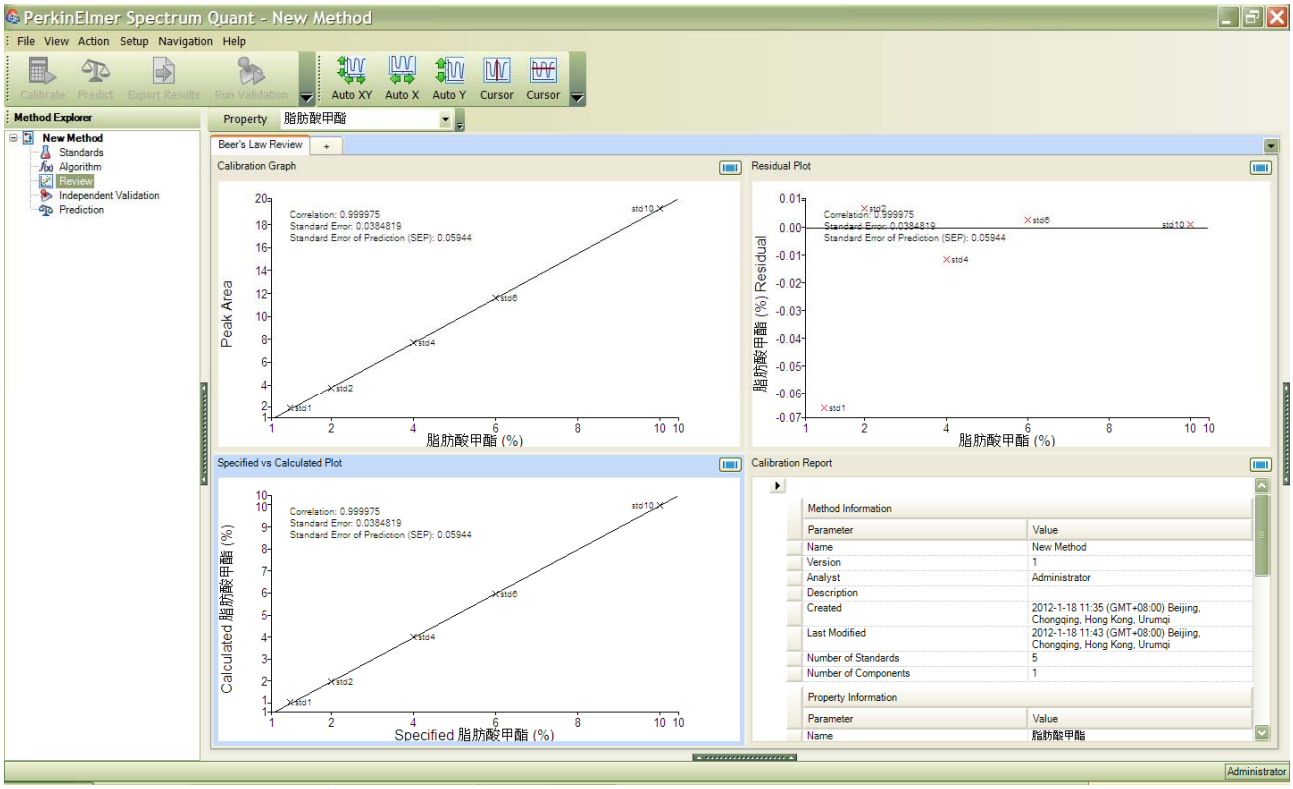


点击校正<Calibrate>



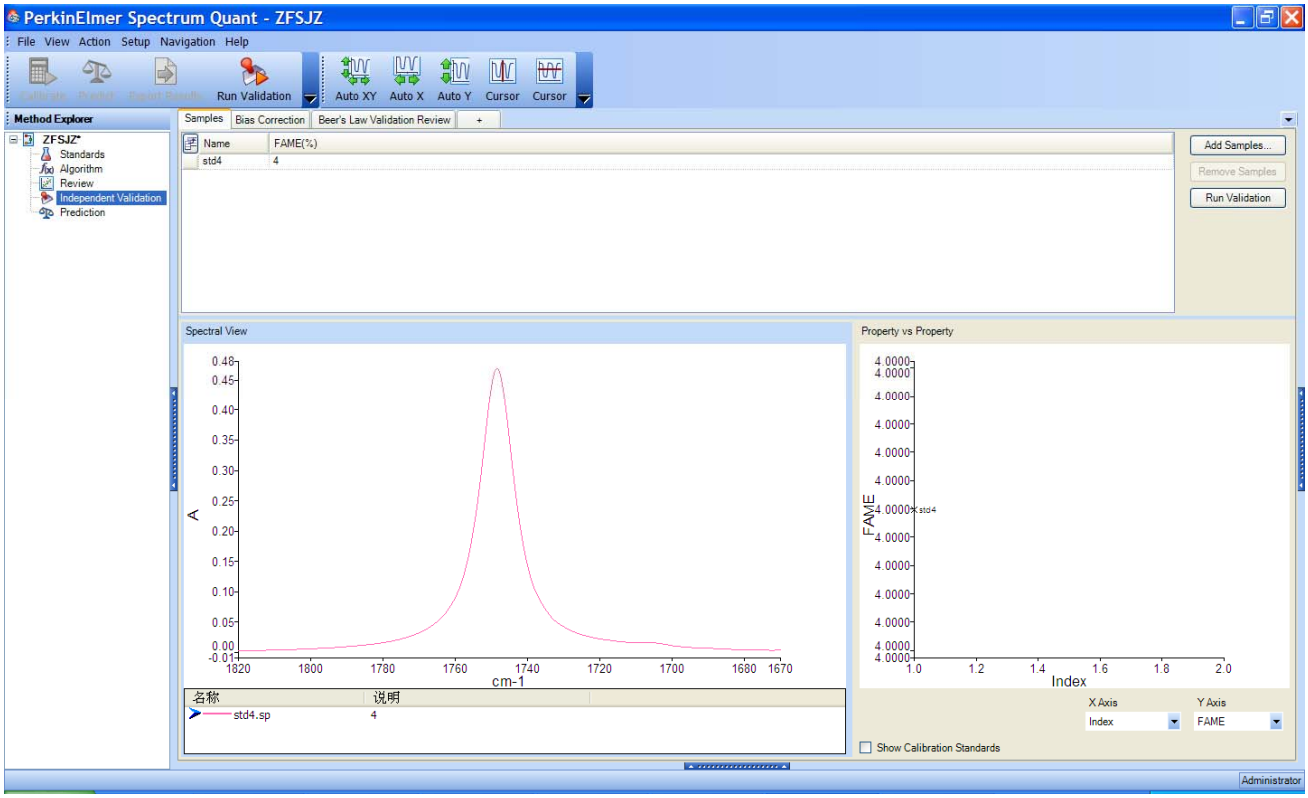
自动到<Review>栏，主工作区域显示有回归曲线图<Calibration Graph>及残差图<Residual Plot>，图中显瘦有相关系数<Correlation>及标准偏差<Standard Error>及预测标准偏差<Standard Error of Prediction(SEP)>

Correlation: 0.999975
Standard Error: 0.0384819
Standard Error of Prediction (SEP): 0.05944

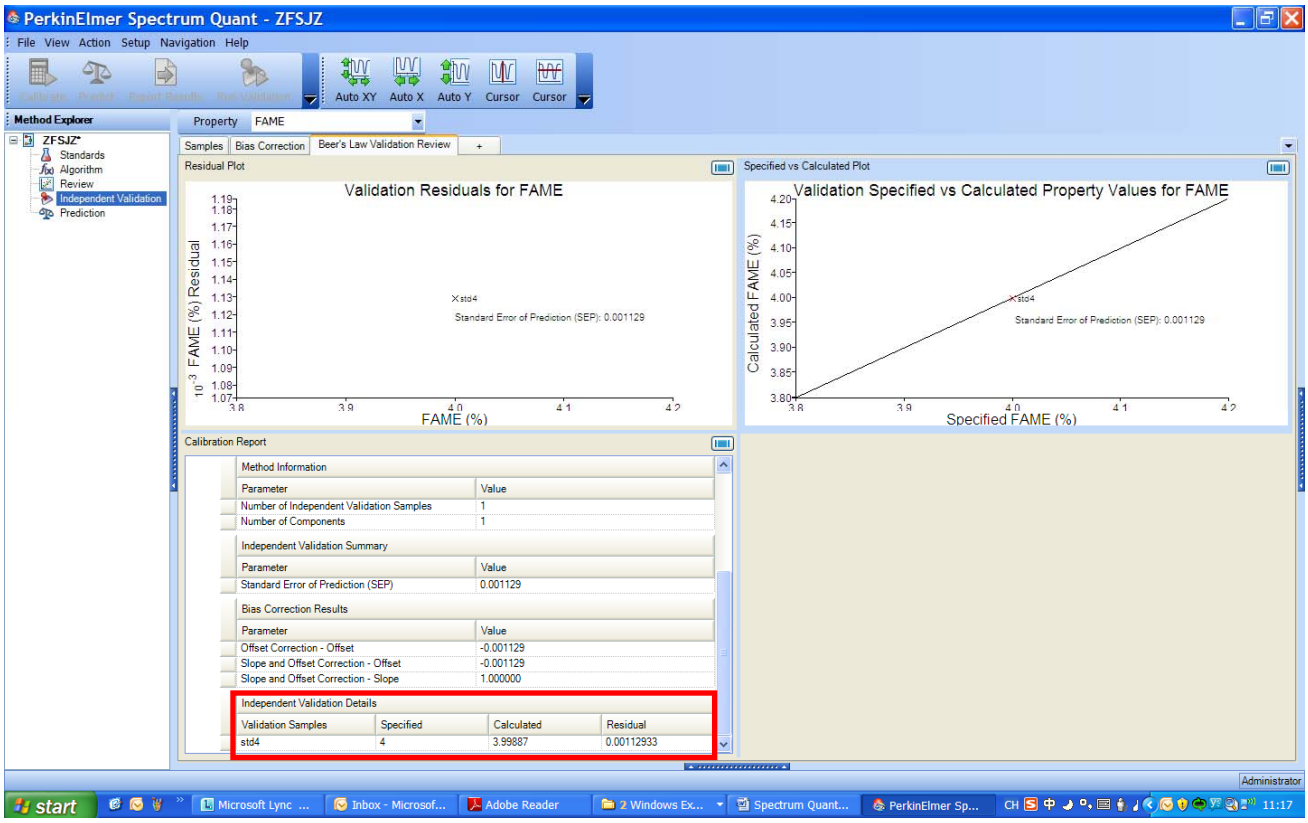


独立(外部)验证——<independent validation>

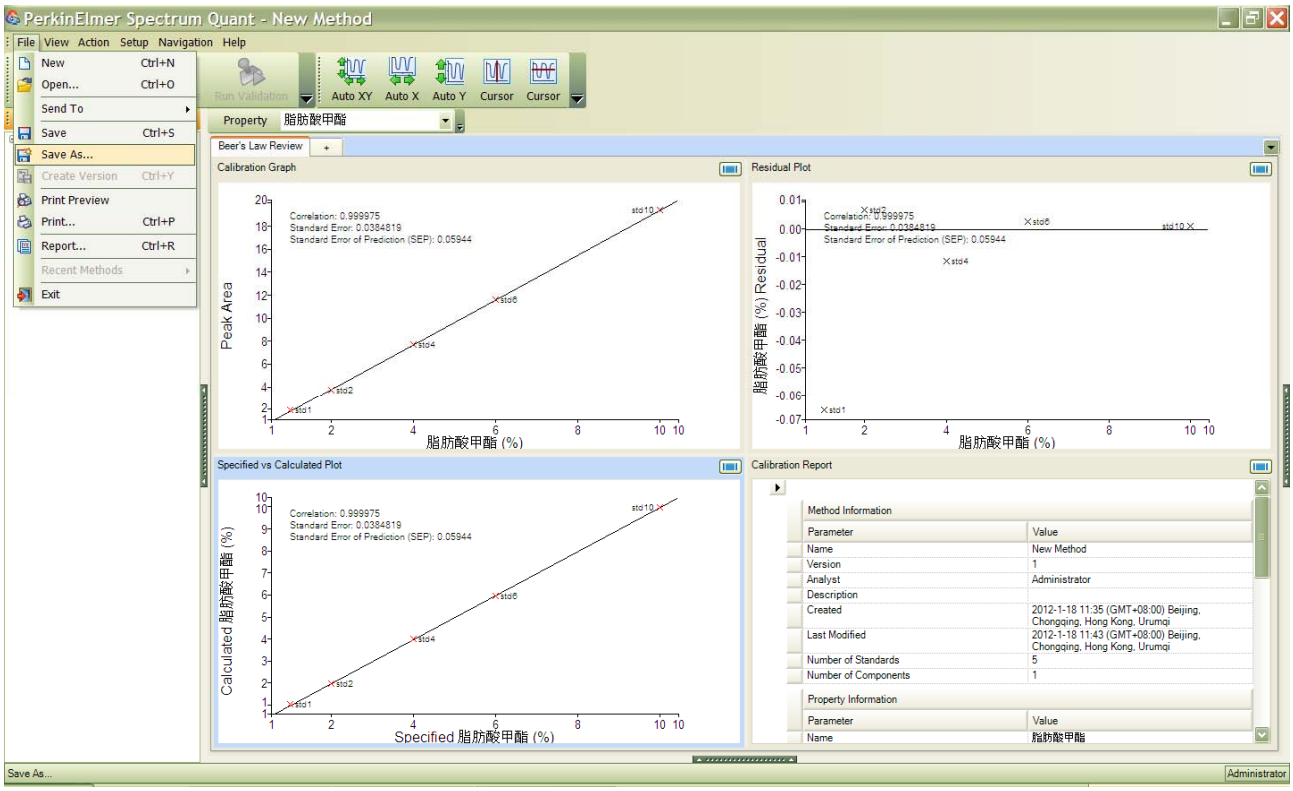
点击添加样品<Add samples>，输入样品对应的浓度值，然后点击执行验证<Run Validation>



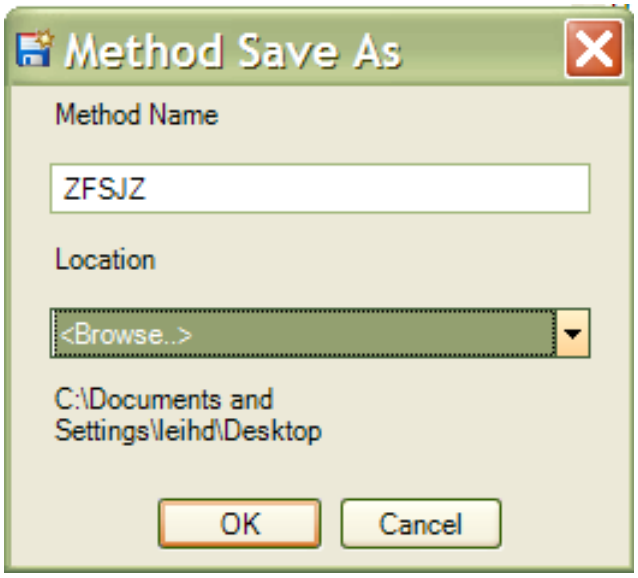
自动到验证结果及报告预览界面<Beer's Law Validation Review>，有残差图<Validation Residuals>，指定值跟计算值相关图<Validation Specified vs Calculated Property Values>和验证报告<Calibration Report>，其中有预测标准偏差<Standard Error of Prediction(SEP)>



如果验证的结果在可接受范围之内、工作曲线可以工作，点击文件<File>——另存为<Save As>，保存方法文件（建议校正过之后再保存）

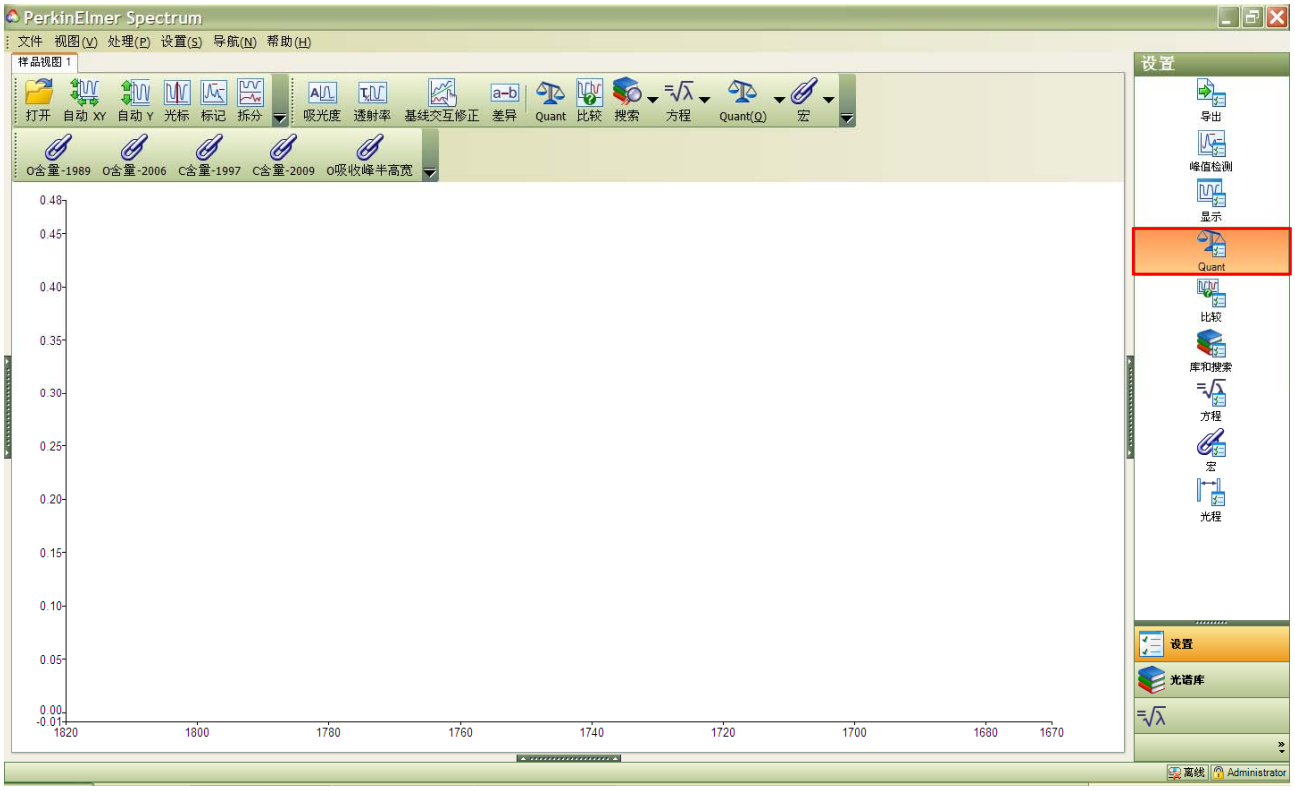


(若第一步没有输方法名称)输如方法名称，选择存储路径，点击 OK，方法文件存为后缀为.qmd 的文件

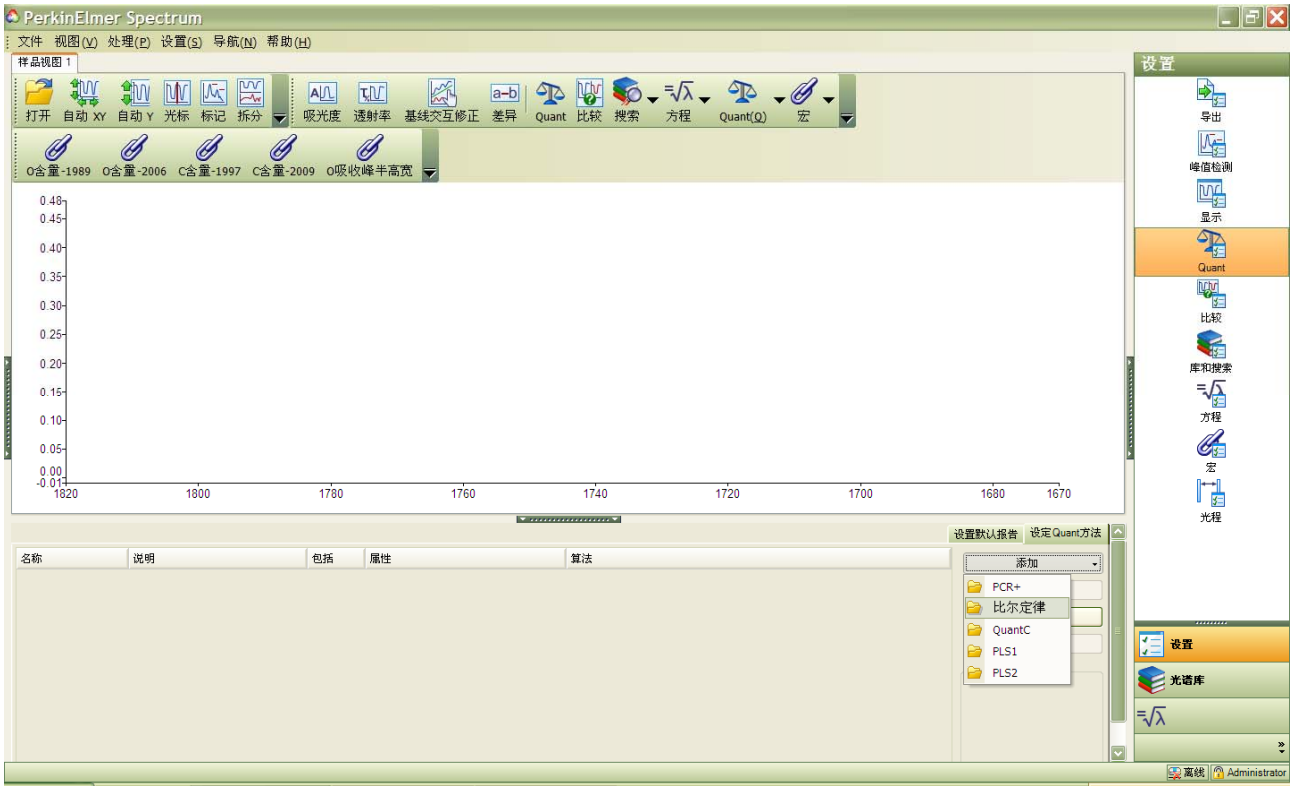


在 Spectrum 仪器主控制操作软件中添加已经建立好的定量方法，点击<设置>——<Quant>

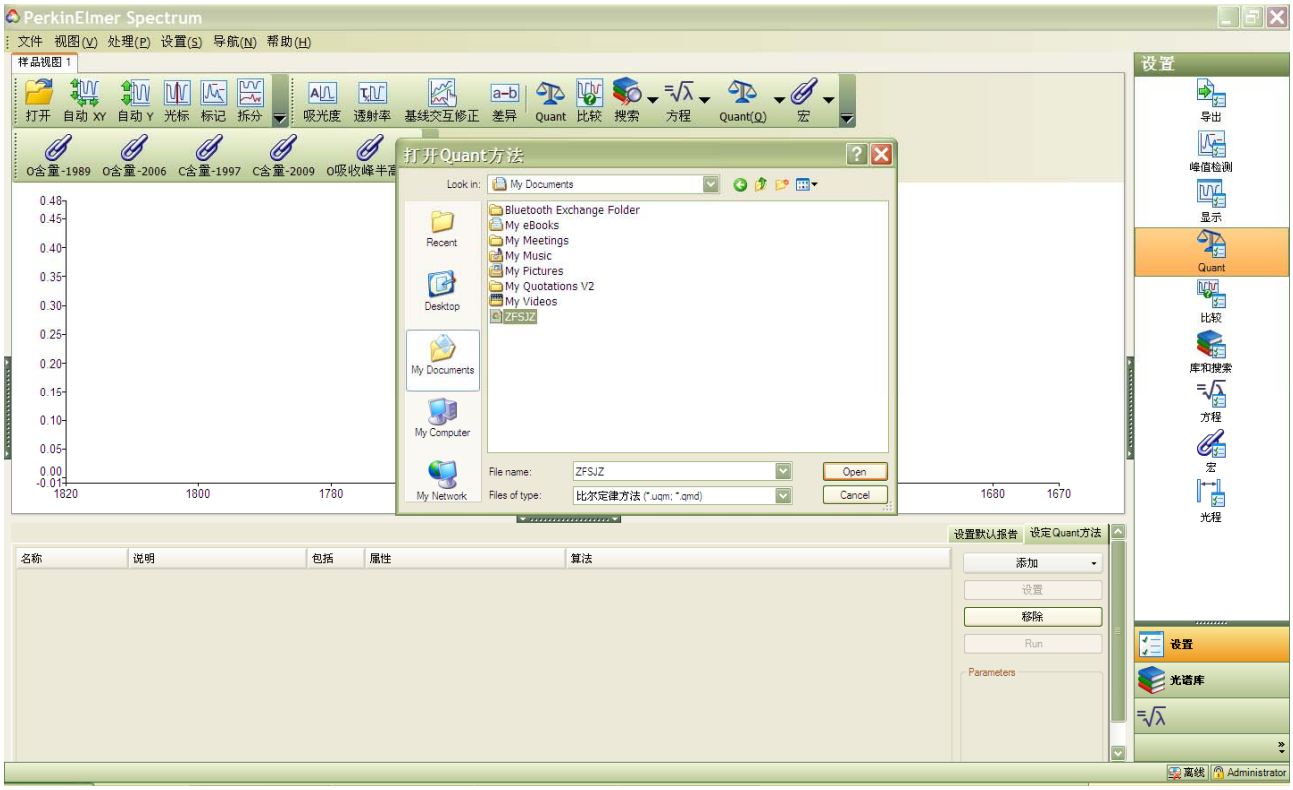
或右侧设置项中的<Quant>

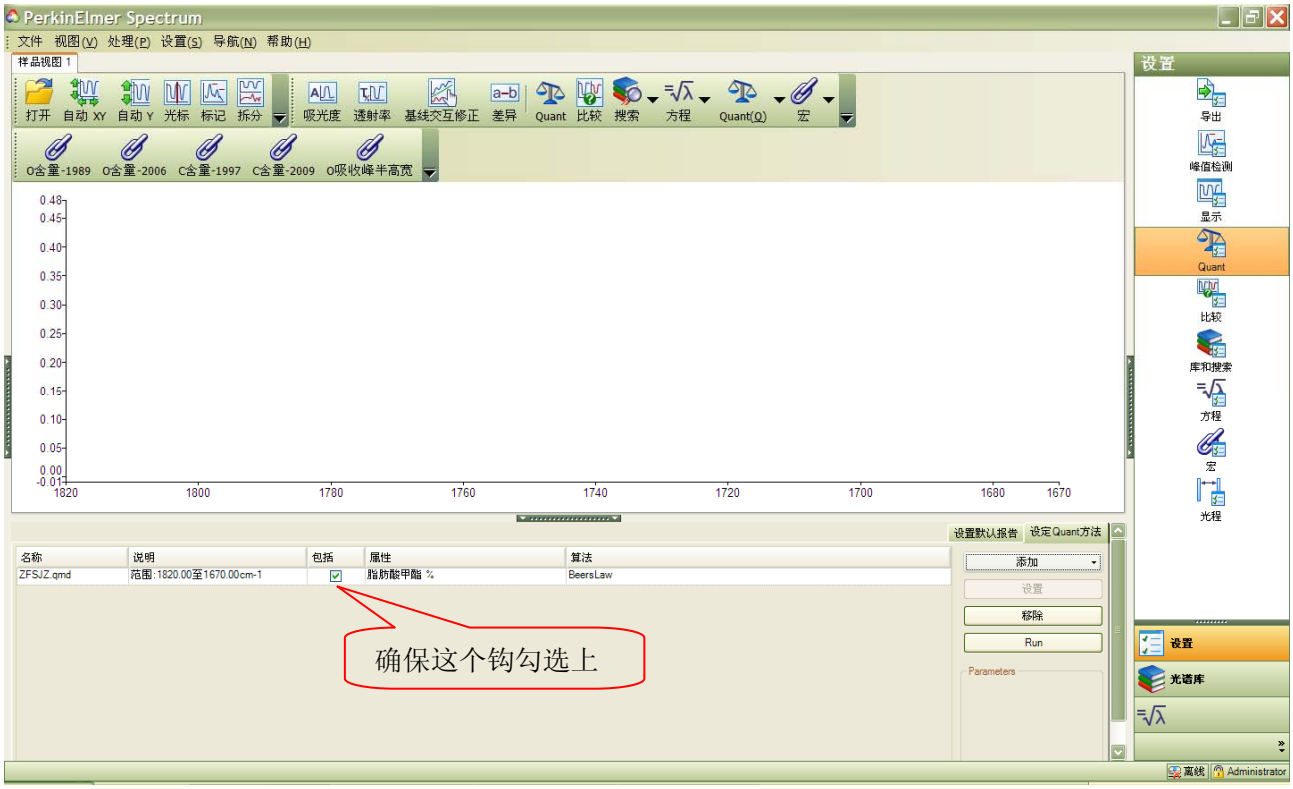


点击<添加>——<比尔定律>

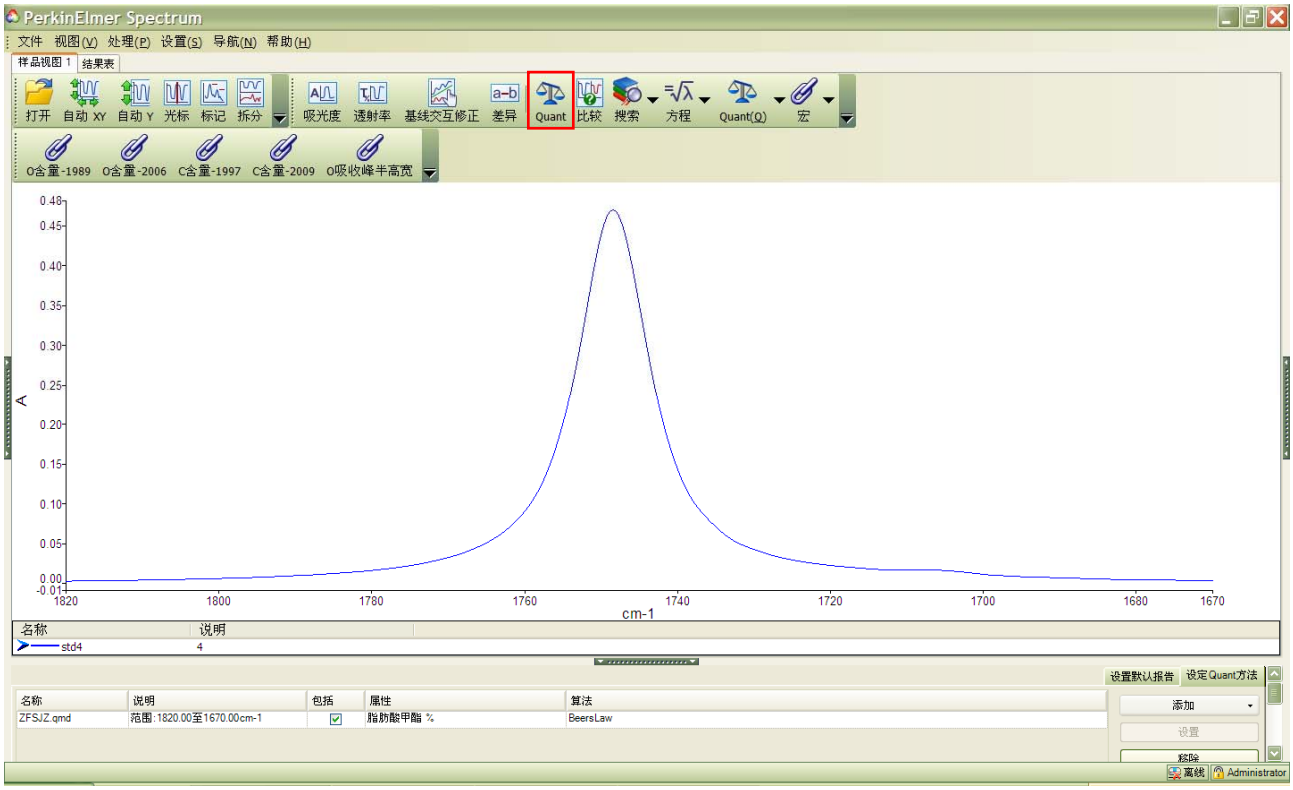


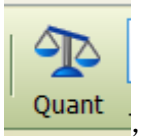
找到存储的方法文件<ZFSJZ>，点击<Open>



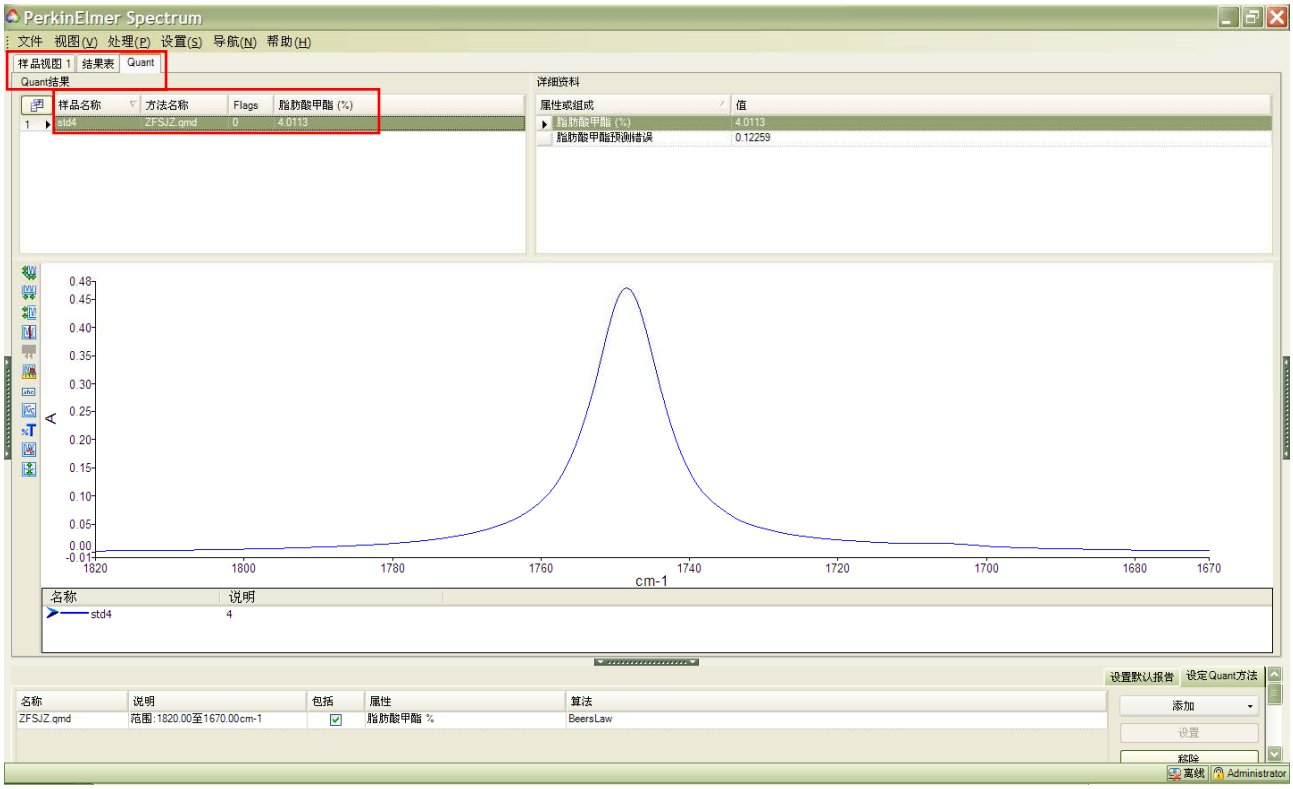


用 Spectrum 软件控制仪器扫描一个或多个待测样品的光谱图，或者打开一个或多个事前已经扫描好的待计算样品的光谱图，纵坐标单位以吸光度 A 显示



点击<Quant> 

，即在<Quant>或者<结果表>中得到计算结果


PerkinElmer Spectrum
文件 视图(V) 处理(P) 设置(S) 导航(N) 帮助(H)
样品视图 1
结果表
Quant
Quant结果
样品名称
方法名称
Flags
脂肪酸甲酯 (%)
std4
ZFSJZ.qmd
0
4.0113
详细资料
属性或组成
值
脂肪酸甲酯 (%)
4.0113
脂肪酸甲酯预测错误
0.12259
A
cm-1
名称
说明
std4
4
设置默认报告
设定Quant方法
名称
说明
包括
属性
算法
ZFSJZ.qmd
范围:1820.00至1670.00cm-1
脂肪酸甲酯 %
BeersLaw
添加
设置
移除
离线
Administrator