# 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。



PerkinElmer Spect	rum Quant	
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	确定 取消	
Version 10.03.06.0100		
Copyright 2011 PerkinElmer, Inc.		Borkin Elmort
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# 点击<确定>进入软件工作界面

File View Action Setup Navigation Help	
Calibrate Prédict Export Results Run Validation V Auto X Auto Y Cursor Cursor	
Method Explorer Summary	
B S New Method Method Name	
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Review Method Description	
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	Administrator

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>,

Method Explorer	Nandards	
Standards	B     Exclude     IP     Property     Add Standards       atd1     atd2     Rename Property     RenaveStandards	
<ul> <li>Independent Validation</li> <li>Rediction</li> </ul>	ati6 Add Column	•
	Remove Column	
	Cross Validation	

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

Rename Property	X
Property Name	
脂肪酸甲酯	
Units	
%	
OK Cancel	

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

🚳 PerkinElmer Spectru	m Quant - New	Method		
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- 700 Algorithm - 201 Review - ∞ Independent Validation - ∞ Prediction		std2	2	Remove Standards
		std4	4	Add Column -
		std6	6	Add Coldmin
		std10	10	Remove Column
				C VELC

# 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>

🚳 PerkinElmer Spectrum	Quant - New Met	hod	_ = ×
File View Action Setup Navigation	on Help		
Calibrate Predict Export Results	Run Validation	to XY Auto X Auto Y Cursor Cursor 🚽	
Method Ex .	ad calibration model to the s	tandard selected in the method and calibrate it accordingly	
B New Method	Algorithm	and a selected in the method and callorate is accordingly	
Standards	Peerle I mu		
J(x) Algorithm	Decis Law	M	
Independent Validation	Summary		
Prediction	Parameter	Value	
	Property Name	脂肪酸甲酯	
	Units	2	
	Peak Ratio	No	
	Calculation Type	Area	
	Start	1800.00	
	End	1680.00	
	Base 1	1820.00	
	Base 2	1670.00	
This will apply the selected calibration mode	el to the standard selected in the	method and calibrate it accordingly	Administrator

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)>

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	Method Information									
	Parameter		Value							
	Number of Independent \	/alidation Samples	1							
	Number of Components		1							
	Independent Validation S	Summary								
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	Parameter		Value							
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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)



<sup>(</sup>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

🖶 Method Save As 🛛 🔀
Method Name
ZFSJZ
Location
<browse></browse>
C:\Documents and Settings\leihd\Desktop
OK Cancel

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>



### 点击<添加>——<比尔定律>



# 找到存储的方法文件<ZFSJZ>,点击<Open>

PerkinElmer Spectrum	
文件	
	设置
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	🕵 离线 🙆 Administrator



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

