## 新手快速入门之如何使用 CDS 软件来进行校正曲线绘制?

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在上一节内容中,我们学习了如何使用安捷伦 CDS 软件在数据分析界面进行批处理方 法的建立及如何优化积分参数,以及给化合物进行命名定性。接下去在本节中,我们将学 习如何使用 CDS 软件进行校正曲线的绘制,来对样品进行定量分析。在绘制校正曲线之前, 我们需要按照上一节内容所提到的,对样品进行一个批处理,将目标化合物都积分上,然 后确定保留时间以及将所有化合物都命名好。这些步骤都做完后才好进行一个校正曲线的 绘制。

◆样品类型的确认:在初始编辑运行序列的时候,我们可以在序列表中对标样进行标注,并进行标样浓度级别设置,做这一步的好处是方便后续校正曲线的绘制。当然这一步很容易遗忘,不过遗忘了也没关系,后续也可以在绘制校正曲线的时候设置。

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5	<b>√</b>	5		🔵 Sample			Test.amx	1	Inject		1	Use Method		Als	Sample 1		<s></s>
6	<b>√</b>	6		Sample			Test.amx	1	Inject		1	Use Method	1	Als	Sample 2		<s></s>
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◆按照上一节内容所讲,进入批处理界面,选择校正曲线标样第一个,然后可以看到 化合物出峰及名称,然后点击圈出来的"Calibration 校正"按钮,继续点击"General" 后我们可以看到一个外标法和内标法选择,这里我用的是外标法,然后校正曲线级别数根 据你实际走的进行设置,这里走了3个点,那我就把数字改为3。

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◆接下去回到""Calibration 校正"下面的"Compound Table"化合物列表界面, 这里面主要有 5 个地方需要我们填写设置,分别为 1. 化合物浓度单位设置; 2. 曲线纵坐标 参考,可以选择以峰面积,也可以选择以峰高来绘制; 3. 曲线模式,可以选择线性拟合方 式,也可以选择二次拟合和对数/指数拟合方式; 4. 原点设置,可以选择曲线包含原点、忽 略原点以及强制过原点等; 5. 校正级别浓度设置,将曲线浓度从按照高低顺序进行填写。



◆然后下一步点击菜单栏上的"Injection List 进样列表"以及"Calibration Curve 校正曲线"两个选项,调出两个窗口。在"Injection List 进样列表"窗口,我们 看到横线划出两个部分,分别为 Sample type 和 Level,如果一开始在编辑序列的时候忘 记指定了,那就在这里进行设置即可。

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◆以上这些地方都设置完成后,那我们就可以点击上方菜单栏 "Reprocess all",对 曲线进行绘制,随后我们就可以看到校正曲线对话框内就出行绘制好的曲线了。要看完成 的曲线,得选中曲线最后一个级别,否则只显示到你选择的那个 Level 上,这个不影响曲 线和最终结果,只是软件在显示上面的一个表现。同时点击样品部分,就可以查看样品经 校正曲线校正后的结果了。



◆上述内容讲的是外标法的绘制,对于内标法曲线绘制略有区别,首现需要在点击 "Calibration 校正"按钮,继续点击"General"后我们选择内标法。

O External standard	Internal standard	
Number of levels	3	
Curve calculation	From average per level	•
RF definition If you change the RF definition Use the "Clear all calibration"	Response per amount on, you need to clear your calibration curve otherwi " RunType for the 1st standard in the injection list to	▼ ise your results will be v o remove the old calibra
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◆对于多参数,多内标内标法曲线绘制来说也不难,首先在化合物识别的时候全都命 名好,化合物和内标都命名对应的名字,然后进入校正栏下的化合物列表,主要进行以下 设置:1.含量单位设置,内标和化合物都需设置;2.内标确认,将属于内标的化合物都勾 选上,告诉软件这几个是内标物;3.内标含量设置;4.给对应的化合物选择相应用来定量 的内标,剩余操作与外标法一样。

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Chromatograms

以上就是本节使用 CDS 软件绘制校正曲线的全部内容,下一节我们将介绍如何导出定

量及定性报告。