新手快速入门之如何使用 CDS 软件来进行数据处理?

刘炜

(富美实(上海)化学技术有限公司,上海 200000)

在上一节内容中,我们学习了如何使用安捷伦 CDS 软件进行单针运行和序列运行。在本节中,我们将学习如何使用 CDS 软件进行数据分析。在处理数据之前首先要调用序列运行采集的数据,可以通过两个地方进入,一个地方是 Aq 主界面序列表中,需要处理哪个序列的数据就选中,然后点击上方按钮,选择查看选中的数据,紧接着就能进入到数据处理软件中了。

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还有一个地方是控制面板,在左下角选中 Projects,然后在菜单栏中点击 Start Data Analysis,同样可以打开数据分析界面,然后再在数据分析界面中打开要分析处理的数据。 这里建议使用第一种方式,想对来说更加便捷。

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◆进入到 DA 界面后,我们就能看到选择序列中已经采集好的数据了,然后点击上方菜 单栏 "Processing",接下去就开始进行数据处理了。



◆点击"New method",创建一个新处理方法,随之跳出一个方法创建对话框,有多种选择,这里需要注意一下。不同仪器选择的处理方法类型不一样,当使用 HPLC 时,建议选择"3D UV Quantitative";当使用 GC 时,建议选择"GC/LC Quantitative";当使用 GCMS 或者 LCMS 时,建议选择"MS"。

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◆这里以 HPLC 为例,选择"3D UV Quantitative",点击下方"Create method", 此时左下角会出现一个"New method 1",然后鼠标放在上面,右键将采集数据链接到该 处理方法,同时将该方法另存在指定路径并命名,处理方法的后缀为.pmx。



理,如果处理正常的话数据右边会出行一个"✔",如果出行"**X**"、"**!**"或者其余显示,代表数据处理异常,就需要去看一下到底哪里出了问题。



◆第一次链接方法进行了批处理后就相当于给数据都已经进行了自动积分,不过相应 的积分参数都是默认的,我们还需要继续进行优化积分参数,还有包括对化合物进行命名 等等,所以先不急着保存最终结果。接下去就是积分参数优化,可以拖动窗口将批处理方 法界面放大,然后选择我们的校正曲线标样。

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◆选中好标样后我们可以看到具体的出峰及积分情况,对于目标化合物我们是需要它 被积分上,而对于一些杂峰,我们不希望被积分上,这样可以让图谱看起来干净一点。我 们在批处理方法中选择化学工作站积分事件设置,对于多通道信号的,我们可以对通道单 独设置积分参数,像 GC 这种采集只有一个信号的,比如 FID,那我们只需要设置一次。点 击右键可以增减积分事件,里面选择有很多,功能很强大,可以对复杂积分进行参数设置, 感兴趣的小伙伴可以去尝试一下。

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◆上述积分参数设置完成后,点击菜单栏"Reprocess all",用优化后的积分参数对 所有样品进行重新处理。处理完成后进行化合物命名,在色谱图上选择要命名的色谱峰, 然后右键选择"Add peak as compound to method",该保留时间的化合物就加到化合物 列表里面了,然后继续修改化合物名称。多个化合物的重复上述操作即可。

Processing Method								
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Injection Results		Copy t	o clipboard					
Peaks Summary		Export	to file					

◆化合物添加好后我们可以在色谱图上看到化合物色谱峰被一个虚线窗口框起来了, 这个代表你设置的批处理方法将该化合物的出峰 RT 时间锁定在了这段内,倘若你的样品存 在保留时间漂移,那么有可能就出现识别不到目标物的情况,这时候我们需要对化合物列 表里的"Absolute RT window"绝对保留时间窗口进行设置,一般设置 0.1[~]0.3 就足够用 了,可以满足正常的漂移识别。如果设置大了,列如做几十种化合物的,本身峰与峰之间 分离度不大,这个窗口一设大,就很容易识别到其它峰上去了。

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◆全部设置好后,最后再对样品进行一个"Reprocess all",这样色谱图上出峰都有 化合物名称了,然后依次保存批处理方法"Save method"及保存结果数据"Save all results"。

以上便是本节的全部内容,对 CDS 软件样品批处理流程进行了一个演示,有什么不对的地方欢迎大家指正。下一节中我们将学习如何进行校正曲线的绘制。