OpenChrom 软件使用介绍 4-保留指数计算和对比

朱建设

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上次说过 OpenChrom 是一款用于色谱,质谱,光谱等数据处理开源软件。可以处理不 同仪器厂家的数据格式,支持通用格式。可以用于不同的电脑操作系统,例如 Windows, macOS, Linux。前面介绍了初步使用的流程和方法,核对质谱结果,谱库文件检索。 https://bbs.instrument.com.cn/topic/8254675

本篇介绍保留指数文件创建和计算,以及保留指数对比。

1 创建保留指数校正文件

在 Processors 菜单下面的 Create Retention Index File。



图 1 创建保留指数校正文件

但这种创建保留指数校正文件需要许多步骤,需要 Calibration Settings, Open Chromatogram (MSD) Files, Peak Selection, Peak Assignment,需要校验正构烷烃化合物等,比较麻烦繁琐。本篇介绍一张非常简单的创建保留指数校正文件方法。

保留指数校正文件的格式为 XXX.cal。里面内容如下例子:



图 2 保留指数校正文件

可以按照图 2 的格式来建立一个写字板模板。可以增加或删去的正构烷碳数数据。另存 为 XXX.CAL 文件。注意存文件时候,文件类型请选择"所有文件类型",不可以选择"文本 类型"。其实这个保留指数校正文件格式和 Amdis 的保留指数校正文件格式一样的,如果您 有 Amdis 的 RI 校正文件,也可以直接使用。当然也可以使用 Amdis 的 RI 校正文件的建立 方法来建立保留指数校正文件。

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图 3 保存保留指数校正文件

2 保留指数校正文件设置

要使用保留指数校正功能,需要一些相应的设置。点击工具栏的 Preference 或 Window 菜单下面 Preference,进入个性化设置。

路径:

Chromatography/Spectrometry----Calculators>Retention Index>Calculator, 点击, 打开

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图 5 添加保留指数校正

点击 Apply and Close。这样就添加了保留指数校正文件。

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图 6 添加保留指数校正文件

3 数据文件计算保留指数

流程如下:

调用 GCMS 数据文件,参见前面第一篇文章。

峰检出,在色谱上面右键点击,Peak Detector>First Derivative。

峰积分,在色谱图上面右键点击,选 Peak integrator>Peak Integrator Trapezoid。

峰鉴定,在色谱图上面右键点击,选 Peak Identifier>NIST(extern)或 Library File (MS)。

参见前面第一或第三篇文章。

保留指数计算:在色谱图上面右键点击,选 Chromatogram Calculator,选择 Retention Index Calculator (Scan and Peaks)



图 7 保留指数校正计算

这样在左上角的Peak/Scan List 里面就有已经计算的 RI 值了,例如保留时间为10.256min





图 8 保留指数校正计算结果

4 化合物保留指数校对

在左下角的 targets 里面可以看到前面选中的化合物谱库里面的保留指数为 1036,这个极性 WAX 柱子,可以认为此化合物的保留指数符合要求,正反质谱匹配度为 94.9,可以确

认这个检索结果。

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I	Ra.	Name	CAS	Match Fa	Reverse	Match Fa	Reverse	Probability	Formu	SMIL	InChl	Mol Weig	Excact M	Identifier	Miscellaneous	C Contribut	Retention Ind
	Ŷ	🔋 Butanoic acid, eth	105-54-4	94.900	94.900	0.000	0.000	-1.000				0.000	0.000	NIST (extern)	InLib Factor: N/A	NIST	1036
	Û	Butanoic acid, eth	105-54-4	93.900	95.400	0.000	0.000	-1.000				0.000	0.000	NIST (extern)	InLib Factor: N/A	NIST	1036
	Û	Butanoic acid, eth	105-54-4	92.300	92.500	0.000	0.000	-1.000				0.000	0.000	NIST (extern)	InLib Factor: N/A	NIST	1036
	Ŷ	Butanoic acid, eth	105-54-4	91.700	92.100	0.000	0.000	-1.000				0.000	0.000	NIST (extern)	InLib Factor: N/A	NIST	1036
	Û	Butanoic acid, eth	105-54-4	91.600	91.600	0.000	0.000	-1.000				0.000	0.000	NIST (extern)	InLib Factor: N/A	NIST	1036
	Φ	Propanoic acid, 2	97-62-1	80.500	81.500	0.000	0.000	-1.000				0.000	0.000	NIST (extern)	InLib Factor: N/A	NIST	961
		in Propanoic acid, e	57-02-1	00.500	00.000	0.000	0.000	-1.000				0.000	0.000	HIST (extern)	India factor. Ny A	NIST	
															1		
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图 9 保留指数校正计算结果和谱库保留指数对比

5 关于检索结果里面的化合物保留指数使用柱子极性的选择

对于 NIST Search 检索,在 Options 菜单选择 Library Search Options。



图 10 NIST Search 结果的柱子极性选择

Library Se	earch Opt	ions					\times
Search	MS/MS	Libraries	Automation	Limits	Constraints	RI (GC)	
Spec	ctrum Sear dentity Normal	ch Type <u>S</u> imilarity ~	/ Precurs	or MW			
Spec	everse Sea atch Ion M	arch lode (Tande	⊡ <u>P</u> enalize m)	rare com	pounds		
● De ○ InC	fault O	Fast C	Off OMV	V 1		Ì	14
	blank :	= match sea	rch spectrum	InChIKey	' -7/	1/	r
O V	ther Optior] <u>A</u> utomatio	ns on	Auto <u>R</u> ep	ort	77/	3	
	Apply Lim	nits	Use Cons	straints			
Struc ☑ M	cture Simila atch Numł	arity Search ber of Rings	Options	Show Hor	mologues		
1	\Box		C	Ж	Cancel		Help

图 11 NIST Search 结果的柱子极性选择

在 RI (GC)下面打勾,根据实际使用的柱子,选择柱子极性,非极性 (例如 DB-1), 弱极性 (例如 DB-5)或极性 (例如 DB-Wax)。

Tury De	earch Opt	ions					X
Search	MS/MS	Libraries	Automation	Limits	Constraints	RI (GC)	
Use Mat Selec St St	Retention ch Factor o ct RI Colur andard No emi-Standa andard Po	Indices (RI correction nn Type for on-Polar (e.g ard Non-Pol lar (e.g. DB) comparison Searching or g. DB-1) ar (e.g. DB-5) -WAX)	for Lib. S Displayin	earch Ig	Þ	7/
□ Colu	umn type s other non-	pecified in s -polar colun	search spectru nn type data if	ım will ov f selected	erride selectio I non-polar typ	n ve data is	V
Colu Use abse Use colu	other non- ent r library spe mn type	pecified in s -polar colun ectra with u	search spectru nn type data if nspecified col	ım will ov f selected umn type	erride selectio I non-polar typ assumed to I	n e data is have selecte	ed
Colu Use abse Use colu	other non- ent r library spe mn type	pecified in s -polar colun ectra with u	search spectru nn type data if nspecified col 10	um will ov f selected umn type	erride selectio I non-polar typ assumed to t	n oe data is have selecte	ed
☐ Colu ✓ Use ✓ Use ✓ colu RI tole RI pen	other non- ent r library spe mn type rance alty rate	pecified in s -polar colun ectra with u	search spectru nn type data if nspecified col 10 Average	um will ov f selected umn type	erride selectio I non-polar typ assumed to h	n e data is have selecte	ed
 Colu Use abso Use colu RI tole RI pen 	umn type s other non- ent r library spe mn type rance alty rate	pecified in s -polar colun ectra with u	search spectru nn type data if nspecified col 10 Average	um will ov f selected umn type	erride selectio I non-polar typ e assumed to I	n he data is	ed

图 11 NIST Search 结果的柱子极性选择

这样才能在检索结果里面看到检索到的化合物的谱库保留指数了,就可以用于结果对比。

6 其它

可以在文件检索下面的 penalty calculation 选择 Retention Index。

	Preferences						- 0 ×
	type filter text Chromatography/Spectrometry	File Identif	ier				
	Baseline Detector	Mass Spectru	ım Libraries				^
	> Calculators > Classifier	Name	Туре	File Name	File Path		Add DB (File)
	> Converter	DEFAULT	Default	nist.db	C:\NIST20\MSSEARCH\mainlib\nist.db		Add DB (Directory)
	> Filter						Remove
	 Identifier Identifier (CSD) 						Remove All
	✓ Identifier (MSD) > Base/Mol Peak Classifie	Limit Match F	actor	80.0			
	CDK Identifier Support	Use search	n pre-optimization				
	Manual Peak Identificat	Threshold pro	e-optimization (0 -	1) 0.1 Euclidean Dict	3860		
	> NIST (extern) - Installati Peak Identifier Templati	Number of Ta	argets	3	unc		
	Peak Numerator Peak Review Template	Min Match Fa	ictor	80.0			
	Peak Review UI [Templa	Min Reverse	Match Factor	80.0			
	> Identifier (WSD)	Delta Calcula	tion	None			~
	> Integrator MS Comparison	Delta Windo	N	Retention Time	e [ms] a [min]		
	> Peak Detector > Process	Penalty Calcu	lation	Retention Inde	e (min) ex		
	> Quantifier	Penalty Wind	ow	0.0			
	> Settings	Penalty Level Max Penalty	Factor	20.0			
	> General > Install/Update	_					
	SWTChart	Use norm	alized scan	Sum			~
	< >		incload of coanc	Jun			~
						10	Apply and Close Cancel
				_			
				图	12 文件检索使用 RI 7	秋 验	
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