# Waters<sup>™</sup>

#### 应用纪要

# 在分析方法的开发中使用Empower™样品组 生成器自动创建色谱方法

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#### 摘要

本技术简报展示如何在基于系统性筛选策略执行的方法开发中使用Empower™样品组生成器(SSG)软件自动创建色 谱方法。本实验研究采用配备PDA和ACQUITY™ QDa™质谱检测器的Arc™ Premier系统进行。使用Empower™色 谱数据软件(CDS)进行数据采集和分析。

#### 优势

- 使用Empower样品组生成器(SSG)自动且快速地创建Empower仪器方法、方法组和样品组方法,以便在 Waters ACQUITY™LC仪器、光学检测器和ACQUITY QDa质谱检测器上执行分析
- 确信所有色谱运行均使用正确创建的方法完成

## 简介

分析方法的开发是一个复杂的过程,需要筛选多种色谱参数才能获得分离效果理想并且稳定耐用的方法。系统性 筛选策略分三个阶段完成方法开发,包括探索、筛选和优化步骤<sup>1-2</sup>。 分析人员会在整个分析过程中系统地评估影 响选择性和分离度的关键因素,并需要精心创建许多色谱方法。 Empower样品组生成器(SSG)软件可针对多种变量自动创建色谱方法<sup>3</sup>。 根据实验设计,在样品组方法中自动创建 和构造Empower方法组和仪器方法,作为准备运行的进样序列。使用Empower SSG,可减少时间和抄录错误 ,确保所有色谱运行均按照正确创建的方法完成。

本技术简报展示如何在方法开发工作流程中使用Empower样品组生成器(SSG)自动且快速地创建色谱方法。我们 采用系统性筛选策略开发一种分析盐酸萘甲唑林和马来酸非尼拉敏活性药物成分(API)及其相关物质的方法。使用 Empower SSG创建运行筛选和优化研究所需的色谱方法。

实验

#### 样品描述

按照之前所述的方法制备包含盐酸萘甲唑啉和马来酸非尼拉敏API及其相关物质的混标溶液<sup>2</sup>。

质谱条件

液相色谱系统:	Arc Premier系统,带色谱柱管理器(主动式)、 PDA和ACQUITY QDa质谱检测器
样品瓶:	LCMS最大回收样品瓶,容积2 mL,P/N:600000670CV
色谱柱:	所有色谱柱均为4.6 x 100 mm,2.5 μm,柱温40 ° C
	XSelect™ Premier CSH™ C <sub>18</sub> (P/N: 186009873)
	XSelect Premier CSH苯己基柱(P/N: 186009890)
	XSelect Premier HSS T3 (P/N: 186009859)
	Atlantis™ Premier BEH™ C <sub>18</sub> AX (P/N: 186009397)
流动相:	A: 1%甲酸水溶液

	B: 1%氢氧化铵水溶液
	C: 水
	D1: 乙腈
	D2:甲醇
流速:	1.0 mL/min
进样体积:	5.0 μL
清洗溶剂:	清除/样品清洗液: 80:20水/甲醇
	密封清洗液:90:10水/乙腈
检测:	UV 260 nm

## 梯度表

	时间 (min)	流速 (mL/min)	%A	%В	%C	%D
1	初始	1.000	10.0	0.0	85.0	5.0
2	10.00	1.000	10.0	0.0	0.0	90.0
3	11.00	1.000	10.0	0.0	0.0	90.0
4	11.10	1.000	10.0	0.0	85.0	5.0
5	15.50	1.000	10.0	0.0	85.0	5.0

#### 数据管理

色谱软件:

Empower<sup>™</sup> 3 Feature Release 5Service Release 5 (FR5 SR5),用于数据采集和分析。

Empower样品组生成器是Empower色谱数据软件(CDS)选配的插件<sup>3</sup>。

## 结果与讨论

我们采用系统性筛选策略开发出一种分析盐酸萘甲唑啉、马来酸非尼拉敏及其相关物质的方法<sup>2</sup>。将Arc Premier 系统与色谱柱管理器和溶剂选择阀集成,可实现色谱柱和有机溶剂的自动切换。

#### 筛选

在筛选阶段,使用乙腈和甲醇溶剂测试采用不同填料的色谱柱。使用Empower SSG软件按照下述步骤创建运行筛 选研究所需的色谱方法(仪器、方法组和样品组方法)。

- 通过加载包含溶剂和色谱柱的逗号分隔值(CSV)文件,将实验设计导入Empower SSG(图1)
- 从Empower项目加载一个基本样品组方法到Empower SSG,其中包括方法组和仪器方法以及分析的系统配置 ,并配置仪器组件(图2)
- 将Empower中溶剂(图3)和色谱柱(图4)设置相关的因素映射到泵和色谱柱管理器模块
- 最终的生成设置包括进样组、平衡时间和方法名称(图5)

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图1.使用Empower SSG创建色谱方法。导入溶剂和色谱柱筛选的实验设计。

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ACQ-QDa (no settings)	A	С	С	6		
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图2.*Empower SSG*。根据需要加载基本样品组方法并配置仪器组件设置。ACQUITY rQSM泵设置:强溶剂和弱溶剂管路、用于强溶剂的"D-切换"、AutoBlend与储备溶剂 管路A。

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图3. Empower SSG。有机溶剂设置: 泵和强溶剂管路。

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   | Value Position         2         1         Column 1         30.00           2         Column 2         30.00         2         Column 2         30.00  | ACQ-CM         1         Column 1         30.00           tting         Valve Position         2         Column 2         30.00  |
| 4 Column 4 V 30.00   
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   |   
  | 1010 00.00   | stom Field None V 3 0.00   | 3 3 Column 3 3 30.00  | Valve Position         2         2         Column 2         30.00           tom Field         None         3         Column 3          30.00   
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  | ALUR-LM         1         Column 1         30.00           ting         Valve Position         2         Column 2         30.00           stom Field         None         3         Column 3         30.00  | Mule         Auxeum         1         Column 1         30.00           ting         Valve Position         2         Column 2         30.00           stom Field         None         3         Column 3         30.00   | Value         Value <th< td=""><td>Value Position         2         Column 1         30.00           stom Field         None         3         Column 3         30.00</td><td>aule         AUQ+CM         1         Column 1         30.00           ting         Valve Position         2         Column 2         30.00           itom Field         None         3         Column 3         30.00</td><td>ACQ-CM         1         Column 1         30.00           tting         Valve Position         2         Column 2         30.00           stom Field         None         3         Column 3         30.00</td><td>ACQ-CM         1         Column 1         30.00           tting         Valve Position         2         Column 2         30.00           stom Field         None         3         Column 3         30.00</td><td>ACQ-CM         1         Column 1         30.00           tting         Valve Position         2         Column 2         30.00           stom Field         None         3         Column 3         30.00</td><td>Value         Value         <th< td=""><td>ACQ-CM         1         Column 1         30.00           tting         Valve Position         2         Column 2         30.00           stom Field         None         3         Column 3         30.00</td></th<></td></th<> | Value Position         2         Column 1         30.00           stom Field         None         3         Column 3         30.00  | aule         AUQ+CM         1         Column 1         30.00           ting         Valve Position         2         Column 2         30.00           itom Field         None         3         Column 3         30.00  | ACQ-CM         1         Column 1         30.00           tting         Valve Position         2         Column 2         30.00           stom Field         None         3         Column 3         30.00  | ACQ-CM         1         Column 1         30.00           tting         Valve Position         2         Column 2         30.00           stom Field         None         3         Column 3         30.00  | ACQ-CM         1         Column 1         30.00           tting         Valve Position         2         Column 2         30.00           stom Field         None         3         Column 3         30.00   | Value         Value <th< td=""><td>ACQ-CM         1         Column 1         30.00           tting         Valve Position         2         Column 2         30.00           stom Field         None         3         Column 3         30.00</td></th<> | ACQ-CM         1         Column 1         30.00           tting         Valve Position         2         Column 2         30.00           stom Field         None         3         Column 3        
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   | None         2         Column 1         30.00           2         Column 2         30.00           3         Column 3         30.00           4         Column 4         30.00   | Value Position         2         Column 1         0.00           tom Field         None         3         Column 3         30.00           4         Column 4         30.00         30.00  | Valve Position         2         Column 1         2         Store           tom Field         None         3         Column 3         >         30.00           4         Column 4         >         30.00   | Valve Position         2         Column 1         2         Store           tom Field         None         3         Column 3         >         30.00           4         Column 4         >         30.00   
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  | ACQ-CM         1         Column 1         30.00           tting         Valve Position         2         Column 2         30.00           stom Field         None         3         Column 3         30.00           4         Column 4         30.00  | None         1         Column 1         30.00           1         Column 1         30.00           2         Column 2         30.00           3         Column 3         30.00           4         Column 4         30.00  | ACQ-CM         1         Column 1         30.00           tting         Valve Position         2         Column 2         30.00           stom Field         None         4         Column 4         30.00   |
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  |   | 4 Column 4 V 30.00   
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  | 4 Column 4 v 30.00   | Stom Field         None         3         Column 3         50.00           4         Column 4         30.00  | 3         3         Column 3         30.00           4         Column 4         30.00   | Image         Valve Position         2         Column 2         30.00           tom Field         3         Column 3         30.00           4         Column 4         30.00  
   | None         2         Column 1         50.00           2         Column 2         30.00           3         Column 3         30.00           4         Column 4         30.00   | Value Position         2         2         Column 1         0         0.00           tom Field         None         4         Column 3         30.00         4         20.00   | ting Valve Position<br>tom Field None<br>Valve Position<br>tom Field None<br>Valve Position<br>tom Field None<br>Valve Position<br>tom Field None<br>Valve Position<br>Valve Position<br>V | ting Valve Position<br>tom Field None<br>Valve Position<br>tom Field None<br>Valve Position<br>tom Field None<br>Valve Position<br>tom Field None<br>Valve Position<br>Valve Position<br>V | ALU2_M         1         1         Column 1         30.00           ting         Valve Position         2         3         Column 2         30.00           stom Field         None         4         Column 3         30.00   | Value         ALU-LM         1         1         Column 1         30.00           tting         Valve Position         2         3         Column 2         30.00           stom Field         None         4         Column 4         30.00  | Value         ALCACIM         1         1         Column 1         30.00           tting         Valve Position         2         3         Column 2         30.00           stom Field         None         4         Column 4         30.00  | None         1         Column 1         30.00           1         Column 1         30.00           2         Column 2         30.00           3         Column 3         30.00           4         Column 4         30.00  
  | Value Position         2         3         2         30.00           stom Field         None         4         Column 1         > 30.00   | dule         ALC4-CM         1         1         Column 1         30.00           ting         Valve Position         2         3         Column 2         30.00           stom Field         None         4         Column 4         30.00   | ACQ-CM         1         Column 1         30.00           tting         Valve Position         2         Column 2         30.00           stom Field         None         3         Column 3         30.00           4         Column 4         30.00   | ACQ-CM         1         Column 1         30.00           tting         Valve Position         2         Column 2         30.00           stom Field         None         4         Column 4         30.00  | ACQ-CM         1         Column 1         30.00           tting         Valve Position         2         Column 2         30.00           stom Field         None         3         Column 3         30.00           4         Column 4         30.00  | None      
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   |  |  |  |  
   | aule AUQ-UM V 1<br>ting UL D IV 2<br>Column 1 V 30.00   | aure AUG-CM ~ 1<br>ting VL D ::: 2<br>Column 1 ~ 30.00  | uure AUGR⊂MI ✓ 1<br>ting VL D II 2 Column 1 ✓ 30.00  | ting Nut p vi 2 Column 1 V 30.00  |   | aule AUG-CM  1 Column 1  30.00 2 Column 2  30.00 2 Column 2  30.00   
  | ACQ-CM         1         1         Column 1         30.00           time         X         Column 2         X         30.00   | AcQ-CM         1         1         Column 1         30.00           Intrins         2 | Indule         ACQ-CM         1         Column 1         30.00           etting         2         Column 2         V         30.00   | tion 1 Column 1 V 30.00  | AcQ-CM         1         1         Column 1         > 30.00           time         X         2         Column 2         X         30.00  |

图4.Empower SSG。色谱柱选择设置:色谱柱管理器和阀位置。

Empower Sam	ple Set Generator -	SSG_meth dev_me	thods_2023 on Usa	-I-1krltq3 as Syster	n	-	×
Final Generation	on Settings						?
Preparation Informal Number of Preparati 1 Number of Injections 1	tion ions/Experiment s/Preparation						
Insert Injection Pane Injections	At the Beginning	On Instrument Method Change	On Preparation Factor Change	On Sample Concentration Change	Number of Injections		
Blank					1		
System Suitability1							
System Suitability2							
Standard						_	
Equilibration Run Ti 10.00	or will insert an Equilit me (Minutes)	ration line when then	e is a charige in che	nistry between samp	ie lines		
Enter Sample Set M	lethod, Method Set a	nd Instrument Method	d Name				
Sample Set Method	Name	7					
ScreeningStudy							
ScreeningStudy							
	Name						
Instrument Method I		7					
ScreeningStudy							
Instrument Method I ScreeningStudy							

图5.*Empower SSG*。色谱方法的最终生成设置,包括样品前处理信息、进样组(空白、 系统适用性、标准品)、平衡时间和方法名称。

完成最终设置后,Empower SSG根据实验设计自动创建样品组方法,作为准备运行的进样序列(图6)。 Empower会在样品组方法中自动创建仪器方法和方法组以及相关的色谱柱和溶剂。按照Empower用户的指示 ,在运行开始时添加平衡步骤和空白进样。使用Empower SSG可以自动生成色谱方法,减少了手动执行该过程所 需的时间和相关的抄录错误。

X	Plate /Well	# of Injs	SampleName	Function	Method Set / Report or Export Method	Run Time (Minutes)	Column Position	Solvents
1				Equilibrate	ScreeningStudy 1	30.00		
2	1:A,2	1	Blank	Inject Samples	ScreeningStudy 1	15.50	1	Acetonitrile
3	1:A,3	1	APIs/Imp mix 1	Inject Samples	ScreeningStudy 1	15.50	1	Acetonitrile
4				Equilibrate	ScreeningStudy 2	30.00		
5	1:A,3	1	APIs/Imp mix 2	Inject Samples	ScreeningStudy 2	15.50	2	Acetonitrile
6				Equilibrate	ScreeningStudy 3	30.00		
7	1:A,3	1	APIs/Imp mix 3	Inject Samples	ScreeningStudy 3	15.50	3	Acetonitrile
8				Equilibrate	ScreeningStudy 4	30.00		
9	1:A,3	1	APIs/Imp mix 4	Inject Samples	ScreeningStudy 4	15.50	4	Acetonitrile
10				Equilibrate	ScreeningStudy 5	30.00		
11	1:A,3	1	APIs/Imp mix 5	Inject Samples	ScreeningStudy 5	15.50	1	Methanol
12				Equilibrate	ScreeningStudy 6	30.00		
13	1:A,3	1	APIs/Imp mix 6	Inject Samples	ScreeningStudy 6	15.50	2	Methanol
14				Equilibrate	ScreeningStudy 7	30.00		
15	1:A,3	1	APIs/Imp mix 7	Inject Samples	ScreeningStudy 7	15.50	3	Methanol
16				Equilibrate	ScreeningStudy 8	30.00		
17	1:A,3	1	APIs/Imp mix 8	Inject Samples	ScreeningStudy 8	15.50	4	Methanol

图6.在筛选阶段使用Empower SSG软件生成的Empower样品组方法

### 优化

在优化阶段,系统地优化色谱参数以获得所需的分离度和色谱性能。

为了说明如何在优化实验中使用Empower SSG创建色谱方法,我们评估了有机溶剂在10 min内从90%降低到 60%的范围内梯度斜率的影响。方法按照筛选部分所述的步骤创建。将梯度斜率映射到泵和强溶剂百分比,以及 梯度分离中的第2行和第3行(或步骤)(图7)。

## 结论

Empower SSG软件基于系统性筛选策略在方法开发工作流程中自动创建色谱方法。该软件会在样品组方法中自动 创建仪器方法和方法组,作为筛选和优化研究中准备运行的进样序列。自动创建色谱方法大幅减少了抄录错误 ,并且缩短了手动创建这些步骤所需的时间。SSG的使用让我们可以确信,色谱运行都是使用正确创建的方法完 成的。

Save All	Import All					
Category	Module	Setting	Custom Field	SSM		
t slope Pump	ACQ+QSM	Strong Solvent %	None			
the user determine the pr	oportion of Strong solve Factor Values	nts in %. Remaining % dete	Property of	/eak solvents f Strong Solve	ent %	
Pump	✓ Reset	Edit Values Sav	Map to al	Lines		
ACQ+QSM	~ 90.0		Line Num	ber M	ар	_
Strong Solvent %	~ 85.0		Line1			-
Ness	80.0		Line2			-
None	75.0		Line4			-
	70.0		Line5			-
ultiple sample set method	Is (SSI 65.0					_
	60.0					
-						
	Save All Category t slope Pump the user determine the pr ACQ+QSM Strong Solvent % None	Save All     Import All       Category     Module       t slope     Pump       ACQ+QSM       the user determine the proportion of Strong solver       Pump       ACQ+QSM       90.0       Strong Solvent %       90.0       Strong Solvent %       80.0       75.0       70.0       utiple sample set methods (SSI       65.0       60.0	Save All       Import All         Category       Module       Setting         t slope       Pump       ACQ+QSM       Strong Solvent %         the user determine the proportion of Strong solvents in %. Remaining % determine the proportion of Strong solvents in %. Remaining % determine %       Factor Values         Pump       Factor Values       Save All         Pump       Paceet       Edit Values         ACQ+QSM       90.0       85.0         Strong Solvent %       80.0       75.0         None       75.0       70.0         utiple sample set methods (SSI       65.0         60.0       60.0	Save All     Import All       Category     Module     Setting     Custom Field       t slope     Pump     ACQ+QSM     Strong Solvent %     None	Save All       Import All         Category       Module       Setting       Custom Field       SSM         t slope       Pump       ACQ+QSM       Strong Solvent ½       None         the user determine the proportion of Strong solvents in %. Remaining % determines proportion of Weak solvents       Property of Strong Solvents         Pump       Factor Values       Property of Strong Solvent Map to all Lines         ACQ+QSM       90.0       85.0         Strong Solvent %       80.0       75.0         None       75.0       10.0         Utiple sample set methods (SSI       65.0         60.0       60.0	Save All       Import All         Category       Module       Setting       Custom Field       SSM         t stope       Pump       ACQ+QSM       Strong Solvent %       None         the user determine the proportion of Strong solvents in %. Remaining % determines proportion of Weak solvents       Property of Strong Solvent %         Pump       Factor Values       Property of Strong Solvent %         ACQ+QSM       90.0       85.0         Strong Solvent %       80.0       75.0         None       75.0       70.0         Utiple sample set methods (SSI       65.0         60.0       60.0

图7.使用*Empower* SSG在梯度斜率的优化中创建色谱方法。将梯度斜率映射到泵和强溶 剂百分比,并应用于梯度分离中的第2行和第3行。

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特色产品

Arc Premier系统 <https://www.waters.com/waters/nav.htm?cid=135083359> ACQUITY QDa质谱检测器 <https://www.waters.com/134761404> ACQUITY UPLC PDA检测器 <https://www.waters.com/514225> Empower色谱数据系统 <https://www.waters.com/10190669>

720008224ZH,2024年2月

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