





# 四極桿式質譜儀 與 TargetLynx 定量軟體 操作手冊



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# I. 建立專案資料夾 Project 與樣品清單(Sample List)

# 1. 登入並建立專案資料夾 Project



A. 執行 MassLynx 軟體

#### B. 輸入使用者的帳號與密碼

MassLynx L	ogin		
Waters La	boratory Inform	ulics	
Ð	Type a logon nar	ne and password to log in.	
Waters	Logon Name:	GLPuser	
	Password:	•••••	
	<u>D</u> omain	ММ2737	
	Role	Regulated 💌	

C. 登入後跳出提示畫面



D. 選擇 File > Project Wizard。





#### E. 按下 Yes



F. 在 Project name 輸入專案資料夾名稱後,按下 Next

Create Project	
Project name	Pesticides_2016
Description	
Location	D:\ Browse
	< Back Next > Cancel

G. 選擇 Create use the default project as template, 按下 Finish.



# 2. 建立樣品清單 Sample List

A. 按下 按鈕 · 建立新的樣品清單。

🍸 Ma	assLynx - Pesticides_2016 - Training.SP	L										<b>- x</b>	
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B. 在表格空白欄位處,按下滑鼠右鍵,選擇 Add。

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C. 輸入想增加的 Sample List 表格列數,按下 OK。

Samples	×
Number of Samples	OK
50 .	Cancel

D. 選擇 File > Save as,以儲存樣品清單名稱。

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E. 輸入樣品清單名稱後,按下 Save。

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F. 視窗上出現 Project 與 Sample List 名稱即建立完成。

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# II. 切換專案資料夾 Project 與樣品清單(Sample List)

- 1. 切換專案資料夾 Project
- A. 點選 🖆 按鈕。

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B. 按下 Yes。



C. 在左側選擇專案資料夾,按下 OK。

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		Drives:
		OK Cancel

D. 軟體開啟專案資料夾後,會自動開啟此資料夾最後一次執行的樣品清單。

🥐 M	assLynx <mark>- Scott - Huabao.SPL</mark>											<b>- X</b>
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- 2. 切換樣品清單 Sample List
- E. 點選 上按鈕。

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F. 選擇樣品清單,按下 Open。

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#### G. 樣品清單開啟成功

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# Ⅲ. 樣品分析

- 1. 建立儀器方法
- A. 點選軟體畫面左側 Instrument 分頁。

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B. 儀器方法總共有以下三種,請參考**附錄一、儀器方法設定**,依序設定完成。

儀器方法種類	液相層析系統	質譜儀-數據紀錄	質譜儀-大氣游離法
設定按鈕圖示	Inlet Method	MS Method	MS Tune

# 2. 準備質譜儀系統-MS Tune

A. 點選左側 Instrument 分頁裡的 MS Tune,出現 **[**] 視窗。

assLynx - Scott - 2016 Training.SPL										_ <b>D</b> _ X
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Solvent Monitor	3	20160928_003	Default	Default	Default	1:A,4	0.000	Standard	10	×
	4	20160928_004	Default	Default	Default	1:A,5	0.000	Standard	25	×
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	6	20160928_006	Default	Default	Default	1:A,7	0.000	Recovery	25	
MS Method	7	20160928_007	Default	Default	Default	1:B,3	0.000	Analyte		
	8	20160928_008	Default	Default	Default	1:B,4	0.000	Analyte		
	9	20160928_009	Default	Default	Default	1:B,5	0.000	QC		
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B. 點選<sup>●●■</sup> 按鈕,開啟氮氣,檢查 Desolvation(L/Hr)與 Cone(L/Hr)有達到設定值。點選<sup>●●●</sup> 按鈕,開啟氦氣。點選●● 按鈕,開啟電壓,檢查 Capillary (kV)、Cone (V)與 Desolvation Temp (℃)有達到設定值。

Waters Xevo TQ-Smicro	o MS Detector - D:\Scott.PRO\ACQUDB\Default.ipr					x
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ES+ Fluidics Extended			Function	Set	Mass	Span
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Ready			Vacuum	Ok	Operate	A



C. 切換到 Fluidics 分頁,將 Valve Position 轉換成 LC。

Waters Xevo TQ-Smicro MS Detector - D:\Scott.PRO\ACQUDB\Default.ipr					
File View Ion Mode Calibration Gas Vacuum Ramps Setup Acquire	e Help				
🗋 🚅 🔄 🚳 🕪 🌆 🖄 🔛 🛄					
ES+ Fluidics Extended Diagnostics		Function	Set	Mass	Span
		MS Scan 👻	56	391	500
	2	Neutral Gain Scan 👻	391	556.3	3
	3	Neutral Gain Scan 👻	502	1121.9	3
	- 4	Neutral Gain Scan 👻	614	2017.6	0
Status Status			204.0		
	3.98e	4	391.0		<u>x1</u>
40.00 minutes remaining at 5.0 μl/min					
200 μl remaining					
LC Position					
Flow					
Flow Rate 5.0 µL/min					
Fill					
Reservoir B 💌					
Fill Volume 200 → μL					
Wash 3 Times when purging.	2	00.0 300.0	400.0	500.0	600.0
					۲
		Vacuum	Ok	Operate	

#### 其他功能說明:

×	質譜儀內建 Syringe 推送樣品
	質譜儀內建 Syringe 裝填樣品
1947 - C. P.	質譜儀內建 Syringe 清洗置換
Flow Rate	質譜儀內建 Syringe 直接進樣流速
Valve Position	質譜儀流路轉閥:
	Infusion - 只有質譜儀內建 Syringe 推送樣品電噴灑
	Combine- 質譜儀內建 Syringe 推送樣品,並與移動相溶液結合後
	才電噴灑。移動相溶液流速,需在 Console 畫面設定
	(p.23) •
	LC- 將層析系統導入電噴灑
	Waste- 將層析系統導入廢液管
Reservoir	質譜儀內建 Syringe 要抽取樣品的位置
Wash	<b>全</b> 按鈕的清洗次數

# 3. 平衡液相層析系統-Inlet

A. 點選左側 Instrument 分頁裡的 Inlet Method · 出現 记录 視窗。

🥐 M	assLynx - Scott - 2016 Training.SPL										x
<u>F</u> ile	<u>V</u> iew <u>R</u> un <u>H</u> elp										~7
2	; -   🗋 💫 🔒   🎒   🕨		] 🛛 🖉 Short	cut 👌	Queue 🖉	Status					
				Qu	eue Is	Empty					
ŧ	Instrument 🥥	Spec	Samples <del>+</del>								
ē	instrument •		File Name	File Text	Inlet File	MS File	MS Tune File	Bottle Inject Volume	Sample Type	Conc A	Quan 🔺
tru		1			Default	Default	Default	0.000			
Ins		2						0.000			
ŝ	Inlet Method	3						0.000			
8		4						0.000			
⊢	(B)	5						0.000			
č		6						0.000			
F	Solvent Monitor	7						0.000			
be la	V	8						0.000			
	TETETE	9						0.000			
×	MS Method	10						0.000			
č	mo method	11						0.000			
<u>ب</u>		12						0.000			
- <del>6</del>		13						0.000			
-	<b>v b</b>	14						0.000			
	System Status	16						0.000			
		17						0.000			
	🔵 Ready	18						0.000			
		19						0.000			+-
		20						0.000			+
		•									•
Ready	/				Not	Scanning		0:0 On	ly Batch Shutdow	n Enabled	1

B. 點選 阅 很 的 · 選擇液相層析方法 · 按下 Open 開啟 ·



# C. 按下 按鈕,執行流速與移動相起始比例。

🚓 TEST.wvhp, TEST.acn	n - Inlet Method					x					
File View Tools L	C Acquity Sampler He	lp									
🗅 🗳 🖬 🎒 🍊	û - He 🖌 🛛 🖉 🔧	) 🗄 🦃									
70	Status										
Status ACQUITY Additional Status Solvent Levels											
otatab	- Indicators	Pumps									
	🔵 Running	🝈 Time (mins):	0.00	3	70.0 %						
Inlet	🔵 Pump On			۵	30.0 %						
-	Inject Cycle	Flow (ml/min):	0.00	周	0.0 %						
Autosampler	🔵 Ready										
Autosampier	单 ок	🥝 Pressure (psi):	-10	6	0.0 %						
	Detector										
Acquity CM	Scan:	Mode: Idle									
For Help, press F1											







E. 出現W视窗·點選左側泵浦選項·確認壓力差值 Delta 小於 50psi·即代表液相層析系統平衡穩定。

Console (Local) - [Binary So	lvent Manager]			_ <b>D</b> _ X							
System Binary Solvent Manager Interactive Display Performance Sample Manager FTN	Control Configure Maintai	n Troubleshoot Help	• Power • Flow								
TUV Detector     Xevo TO-Smicro MS Detec	conditions		performance								
IntelliStart	6604 psi	<u>A1</u> <u>70.0</u> %	BSM Total volume pumped	Flow							
<ul> <li>Manual Optimization</li> <li>MS Display</li> <li>Interactive Fluidics</li> </ul>	0.300 mL/min	<u>B1</u> <u>30.0</u> %	51.7 <mark>64 L</mark>	Stree Elever							
Column Manager	Degasser:	Vent Valve:	pressure ripple (psi, 1 min) Minimum Maximum Delta								
- Maintenance Counters	0.43 psi[a]	System	6602 6611 9								
Logs				Home							
	DOM Custom Dec										
System Status	6800.00			Realtime							
	BSM Flow Rate			Full View							
	붙 0.305-										
	0.295 -			▼ Unzoom							
	-5.00 -4.00 -3.00 -2.00 -1.00 Minutes										
	<										
				.::							



### 4. 編輯樣品清單

A. 分別在 Inlet File、MS File、MS Tune File 欄位點滑鼠左鍵兩下,即可選擇儀

器方法。

🍸 Ma	assLynx - Scott - 2016 Training.SPL										×	
<u>F</u> ile	<u>V</u> iew <u>R</u> un <u>H</u> elp										-T	
2	- 🗋 💺 📙 🕼 🕨		🖉 Shor	tcut 🔓	Queue 🖉	Status						
	Queue Is Empty											
ŧ	Instrument 2	Spec	trum Chro	matogr	ram Map	Edit 🗸	Samples 🕶					
e E			File Name	File Tex	t Inlet File	MS File	MS Tune File B	ottle Inject Volume	Sample Type	Conc A	Quan 🔺	
tru		1			Default	Default	Default	0.000				
Ins		2					,	0.000				
	Inlet Method	3						0.000				
		4			<b></b>	左鍵點	城下	0.000				
Ĕ	(PA)	5						0.000				
ž	45	6					1	0.000				
Ľ,	Solvent Monitor	7						0.000				
ber		8						0.000				
ō	TTTT	9						0.000				
S		10						0.000				
Â	MS Method	11						0.000				
L Z		12						0.000				
get		13						0.000				
	$\mathbf{O}$	14						0.000				
<b>-</b>		15						0.000				
	System Status	16						0.000				
	Deadu	17						0.000				
	- кеаду	18						0.000				
		19						0.000				
		20						0.000				
Pearle		•			N-+	Comming		0	ly Datab Chutal	uun Enabled		
Ready					Not	scanning	(	On On	ly Batch Shutd	own Enabled	1.	

B. 在 Bottle 欄位按下滑鼠右鍵,選擇 Auto Sampler Bed Layout。



C. 在樣品盤示意圖點選樣品位置,按下滑鼠右鍵,選擇 Replace。

AutoSampler Bed Layo	out X
2 Plate Bed	<u>3</u> ₩= 3₩E 3 <sub>4=</sub>
ANSI-48Via	l2mLHolder
ANSI-48Via	l2mLHolder
Plate: 1	
1 2 3 4 5 6 7 A 🏶 🏶 🏶 🏶 🏶 🏶	8
	Insert Add
E • • • • • •	Replace
	Select all Vials Un-select All Vials

D. 樣品位置自動填入樣品清單中

🍸 Ma	ssLynx - Scott - 2016 Training.SPL										_	x
<u>F</u> ile	<u>V</u> iew <u>R</u> un <u>H</u> elp											-Y
2	• 🗅 💺 🔒 🎒 🕨		Short	tcut	Queue 🔮	Status						
				Qu	ieue Is	Empty						
🗧 📻 Instrument 🕢 Spectrum Chromatogram Map Edit - Samples -												
ner	Instrument 🕑	· ·	File Name	File Text	Inlet File	MS File	MS Tune Fil	Bottle	Inject Volume	Sample Type	Conc A	Q. 🔺
tru 📲		1			Default	Default	Default	1:A,2	0.000			
suj		2						1:A,3	0.000			
	Inlet Method	3						1:A,4	0.000			
l loo		4						1:A,5	0.000			
Ĕ	(BB)	5						1:A,6	0.000			
č		6						1:A,7	0.000			
Ę	Solvent Monitor	7						1:B,3	0.000			
bei		8						1:B,4	0.000			
0	TTTT	9						1:B,5	0.000			
Xs	MC Mathad	10							0.000			
ž	MS Method	11							0.000			
Ē		12							0.000			
g		13							0.000			
	0 0	14							0.000			
	System Status	15							0.000			
	System Status	16							0.000			
	Ready	17							0.000			
		18							0.000			
		19							0.000			
		•						I				Þ
Ready					Not	Scanning		0:0	Only E	Batch Shutdown	Enabled	1

E. 輸入其他欄位 · 欄位說明如下表

欄位名稱	填入內容									
	素 品 檔 案 名 稱 · 建 議 以 不 會 重 複 的 流 水 編 號 命 名 • 例									
File Name	如:20160928_001、20160928_002等。									
File Text 樣品註解資訊。										
Injection Volume	樣品注射體積(μL)。									
	檔案類型。標準品選擇 Standard;樣品選擇 Analyte;品管標準品									
Sample Type	選擇 QC;回收率樣品選擇 Recovery。									
Conc A/Conc B	標準品濃度或回收率樣品期望濃度。									
Quan Reference	填入 x·此檔案會列入 TargetLynx 計算標準 ion ratio。									

F. 滑鼠左鍵按住下拉,選擇 Fill Series,可連續編號。

🍸 Ma	ssLynx - Scott - 2016 Training.SPL										_ 0	x
<u>F</u> ile	<u>V</u> iew <u>R</u> un <u>H</u> elp											-T
2	- 🗋 💫 🔒 🎒 🕨		Shorte	ut 🔒 Quei	je 🐬	Status						
				Queue	e Is Ei	npty						
t z	Tustument	Spectr	rum Chron	natogram	Map	Edit - S	amples 🗸					
u eu	Instrument 💋		File Name	File Text	Inlet File	MS File	MS Tune F	le Bottle	Inject Volume	Sample Type	Conc A	
- In		1 2	0160928_001		Default	Default	Default	1:A,2	2.000			
nst		2						1:A,3	0.000			
	Inlet Method	3						1:A,4	0.000			
		4		Cut				1:A,5	0.000			
Ĕ	(Egs)	5		Сору				1:A,6	0.000			
ž	(FB)	6		Paste				1:A,7	0.000			
L Y	Solvent Monitor	7		Add				1:B,3	0.000			
ber		8		Incert	Add			1:B,4	0.000			
•	TTTT	9		Insert				1:B,5	0.000			
x X	MC Mathad	10		Fill Down					0.000			
ž	MS Method	11		Fill Series					0.000			
L L	0	12		Clear Sel	octed				0.000			
<u>a</u>		13		Clear Ser	cieu				0.000			
	$\mathbf{\nabla}$	14		Customiz	e Display	/			0.000			
	System Status	15		AutoSam	nler Bed	Lavout			0.000			
	System Status	16		Autoball	pier beu	Layout			0.000			
	Ready	17							0.000			
		18							0.000			
		19							0.000			-
		•							111881			Þ
Ready					Not Sc	anning		0:0	Only Bat	ch Shutdown Er	nabled	<b>%</b>

G. 滑鼠左鍵按住下拉,選擇 Fill Down,可連續編號。

🌱 M	assLynx - Scott - 2016 Training.SPL									_ 0	x
<u> </u>	<u>V</u> iew <u>R</u> un <u>H</u> elp										-7
2	🚔 🔻 🗋 🗞 📕 🎒 🕨 🔲 🔢 🦉 Shortcut 🗟 Queue 🐼 Status										
Queue Is Empty											
Tostrument Spectrum Chromatogram Map Edit - Samples -											
n er	Instrument .		File Name	File Text	Inlet File	MS File	MS Tune File f	Bottle Inject Vo	lume   Sample Type	Conc A	
tru		1	20160928_001		Default	Default	Default	1:A.2	2.000		
Sul		2	20160928_002					Cut			
	Inlet Method	3	20160928_003					Сору			
sioc		4	20160928_004					Paste			
Ĕ	(PB)	5	20160928_005					Add			
ž	6	6	20160928_006					Add			
Ę	Solvent Monitor	7	20160928_007					Insert			
per		8	20160928_008					Fill Down			
0	TTTT	9	20160928_009					Class Salactor			
ŝ		10						Clear Selected	1		
2	MS Method	11						Customize Di	splay		
Ę		12						AutoSampler	Pod Lavout		
ge		13						Autosampier	Bed Layout		
	$\mathbf{\nabla}$	14							0.000		
	Sustan Status	15							0.000		
	System Status	16							0.000		
	Ready	17							0.000		
		18							0.000		
		19							0.000		
		<20							0 0001		F
Ready	1	_			Not Sc	anning	0:	0 0	nly Batch Shutdown	Enabled	1

H. 樣品清單填寫完畢後,按下 按鈕,儲存樣品清單內容。

🌱 Ma	assLynx - Scott - 2016 Training.SPL											x
<u>F</u> ile	<u>V</u> iew <u>R</u> un <u>H</u> elp											-1
2	; •   🗅 🖻 🔒 🎒   🕨		Short	cut 🖣	Queue 🔮	Status						
Queue Is Empty												
Tostrument Spectrum Chromatogram Map Edit - Samples -												
u er	Instrument .		File Name	Inlet File	MS File	MS Tune	File Bottle	Inject Volume	Sample Type	Conc A	Quan Referen	n 🔺
tru		1	20160928_001	Default	Default	Default	1:A,2	2.000	Standard	0.5		
Su]		2	20160928_002	Default	Default	Default	1:A,3	0.000	Standard	2	×	
	Inlet Method	3	20160928_003	Default	Default	Default	1:A,4	0.000	Standard	10	×	
loo		4	20160928_004	Default	Default	Default	1:A,5	0.000	Standard	25	×	
Ĕ	(BR)	5	20160928_005	Default	Default	Default	1:A,6	0.000	Standard	50	×	
ž	(GE)	6	20160928_006	Default	Default	Default	1:A,7	0.000	Recovery	25		
Ę	Solvent Monitor	7	20160928_007	Default	Default	Default	1:B,3	0.000	Analyte			
ber		8	20160928_008	Default	Default	Default	1:B,4	0.000	Analyte			
ō	TTTT	9	20160928_009	Default	Default	Default	1:B,5	0.000	QC			
ιŝ		10						0.000				
Ê	MS Method	11						0.000				
ι Γ		12						0.000				
get		13						0.000				
•	$\mathbf{O}$	14						0.000				
<b>–</b>		15						0.000				
	System Status	16						0.000				
	Ready	17						0.000				
	- Ready	18						0.000				
		19						0.000				
		20						0 000				) )
Ready						t Scanning		0:0	Only Ba	tch Shutdowr	n Enabled 🛛 🖗	ā /

# 5. 執行樣品清單

A. 按住滑鼠左鍵選擇樣品,點選 ▶ 按鈕。

🍸 Ma	assLynx - Scott - 2016 Training.SPL										- <b>-</b> X	
<u>F</u> ile	<u>V</u> iew <u>R</u> un <u>H</u> elp										*/	
2	- 🗅 🗟 🔒 🌗 🕨		🛛 🖉 Short	cut 🔓	Queue 🦉	Status						
	Queue Is Empty											
Ħ	Instrument @	Spect	trum Chroi	natogr	am Map	Edit 🗸	Sampl	es 🕶				
E	instrument 😈		File Name	Inlet File	MS File	MS Tune File	e Bottle	Inject Volume	Sample Type	Conc A	Quan Referen 🔺	
E .	(ZR)	1	20160928_001	Default	Default	Default	1:A,2	2.000	Standard	0.5		
Ins	(FE)	2	20160928_002	Default	Default	Default	1:A,3	0.000	Standard	2	×	
s	Solvent Monitor	3	20160928_003	Default	Default	Default	1:A,4	0.000	Standard	10	×	
8		4	20160928_004	Default	Default	Default	1:A,5	0.000	Standard	25	×	
F ⊢	TTTT	5	20160928_005	Default	Default	Default	1:A,6	0.000	Standard	50	×	
ž		6	20160928_006	Default	Default	Default	1:A,7	0.000	Recovery	25		
ζ.	MS Method	7	20160928_007	Default	Default	Default	1:B,3	0.000	Analyte			
be l		8	20160928_008	Default	Default	Default	1:B,4	0.000	Analyte			
•		9	20160928_009	Default	Default	Default	1:B,5	0.000	QC			
ŝ		10						0.000				
Ê	MS Tune							0.000				
4		坊	主语目力	= 纽建	跸摆槎,			0.000				
đ		JX I.	<i>그 /편</i> 태/그		さ「羊」水」	-11-1		0.000				
•	$\mathbf{O}$							0.000				
<b>-</b>		15						0.000				
	System Status	16						0.000				
	Dandy	17						0.000				
	- Ready	18						0.000				
		19						0.000				
		20						0 000		1		
		•										
Ready					Not	Scanning		0:0	Only Ba	tch Shutdow	n Enabled 🛛 🧏 🖉	



B. 勾選 Acquire Sample Data, 點選 OK

Start Sample List Run	×
D:\Scott.PR0	
Pre-Run ✔Acquire Sample Data Auto Process Samples Auto Quantify Samples Post-Run	Samples From 1 To 9 QCMonitor Enabled Scheduling Priority Night Time Process
User Processes	OK Cancel

C. 綠色方塊圖示表示目前正在分析的樣品。

🌱 Mas	ssLynx - Scott - 2016 Training.SPL										
<u>F</u> ile	<u>V</u> iew <u>R</u> un <u>H</u> elp										
2	- 🗅 🗞 🔒 🎒 🕨		Shorte	ut 🗗	Queue	😼 Status					
201	6 Training - Samples 1 t	o 9: S	ample 1 /	Acqui	ring						
ŧ	Instrument 🕐	Spect	rum Chror	natogr	am Map	Edit <del>•</del>	Sampl	es 🕶			
Ē			File Name	Inlet File	MS File	MS Tune File	e Bottle	Inject Volume	Sample Type	Conc A	Quan Referen 🔺
it.	(PA)	1	20160928_001	Default	Default	Default	1:A,2	2.000	Standard	0.5	
Ë		2	20160928_002	Default	Default	Default	1:A,3	0.000	Standard	2	×
s	Solvent Monitor	3	20160928_003	Default	Default	Default	1:A,4	0.000	Standard	10	×
8		4	20160928_004	Default	Default	Default	1:A,5	0.000	Standard	25	×
	TTTTT	5	20160928_005	Default	Default	Default	1:A,6	0.000	Standard	50	×
х с		6	20160928_006	Default	Default	Default	1:A,7	0.000	Recovery	25	
l <del>2</del>	MS Method		20160928_007	Default	Default	Default	1:B,3	0.000	Analyte		
be		8	20160928_008	Default	Default	Default	1:8,4	0.000	Analyte		
		9	20160928_009	Default	Default	Default	1:8,5	0.000	ųC		
Xs	MS Tupo	10						0.000			
č	MS Ture	11						0.000			
Ę		12						0.000			
B		13						0.000			
Î.	<b>v o</b>	14						0.000			
	System Status	15						0.000			
	System Status	16						0.000			
	Ready	17						0.000			
		18						0.000			
		19						0.000			
		20						0 000			
Ready		start 1	1:0	Only Ba	tch Shutdowr	n Enabled 🏾 🍢 🏿					

# IV.數據處理

# 1. 建立定量數據處理方法-TargetLynx

A. 在樣品清單選擇一筆數據,點選表格上方的 Chromatogram,開啟層析圖。

🍸 Ma	ssLynx - Quantify - Quantify.spl												
<u>F</u> ile	<u>V</u> iew <u>R</u> un <u>H</u> elp									6	1		
2	-   🗅 🗞 🔒   🎒   🕨		Shc	rtcut 🔒 Que	ue ኇ Status								
Queue Is Empty													
Ħ	Target you XS	Spec	trum Chr	omatogram	Map Edit -	Samples -	Samples -						
۲.			File Name	Sample ID	File Text	MS File	Inlet File	Bottle	Inject Volume	Sample	*		
Ľ,		1	ASSAY01	ID	plasma blank	DEFAULT	DEFAULT	1	10.000	Blank			
is I		2	ASSAY02	ID2	0.2pg/ml std	DEFAULT	DEFAULT	2	10.000	Standard			
	Edit Method	3	ASSAY03	ID3	0.5pg/ml std	DEFAULT	DEFAULT	3	10.000	Standard			
1 a		4	ASSAY04	ID4	0.75pg/ml std	DEFAULT	DEFAULT	4	10.000	Standard			
Ĕ		5	ASSAY05	ID5	1pg/ml std	DEFAULT	DEFAULT	5	10.000	Standard			
ž		6	ASSAY06	ID6	2pg/ml std	DEFAULT	DEFAULT	6	10.000	Standard	=		
Ξ	Process Samples	7	ASSAY07	ID7	5pg/ml std	DEFAULT	DEFAULT	7	10.000	Standard			
penl		8	ASSAY08	ID8	10pg/ml std	DEFAULT	DEFAULT	8	10.000	Standard			
0		9	ASSAY09	ID9	15pg/ml std	DEFAULT	DEFAULT	9	10.000	Standard			
S I		10	ASSAY10	ID10	0.3pg/ml QC	DEFAULT	DEFAULT	10	10.000	QC			
i i i	VIEW Results	11	ASSAY11	ID11	2pg/ml QC	DEFAULT	DEFAULT	11	10.000	QC			
Ľ,		12	ASSAY12	ID12	12pg/ml QC	DEFAULT	DEFAULT	12	10.000	QC			
get		13	ASSAY13	ID13	Rat sample 01	DEFAULT	DEFAULT	13	10.000	Blank			
Tar	TrendPlot	14	ASSAY14	ID14	Rat sample 02	DEFAULT	DEFAULT	14	10.000	Analyte			
		15	ASSAY15	ID15	Rat sample 03	DEFAULT	DEFAULT	15	10.000	Analyte			
	0 0	16	ASSAY16	ID16	Rat sample 04	DEFAULT	DEFAULT	16	10.000	Analyte			
t	System Status	17	ASSAY17	ID17	Rat sample 05	DEFAULT	DEFAULT	17	10.000	Analyte			
Sta	System Status	18	ASSAY18	ID18	Rat sample 06	DEFAULT	DEFAULT	18	10.000	Analyte			
	🔴 Not Ready	19	ASSAY19	ID19	Rat sample 07	DEFAULT	DEFAULT	19	10.000	Analyte			
Inte		20	ASSAY20	ID20	Rat sample 08	DEFAULT	DEFAULT	20	10.000	Analyte			
	instrument in standby	21	ASSAY21	ID21	Rat sample 09	DEFAULT	DEFAULT	21	10.000	Analyte	-		
		•	14004200		ID - L 10				10 000	A			
Ready					Not Scanning		0:0	Only Batch SI	hutdown Enable	d 🍢	11.		



B. 在層析圖視窗,點選 按鈕,在 Function 選單選擇成分,在 Channels

滑鼠左鍵點選兩下要開啟的圖檔·點選 Replace trace·按下 OK。

🚎 Chromatogram - [ASSAY02]	
📕 File Edit Display Process Tools Window Help	_ 8 ×
🖆 🖉 😰 📾 🖻 🖻 🔼 🔽 🕰 💽 A 🖷 🛍 Ϋ 🔍 🗘 🖬 🕅	
0.2pg/ml std	
ASSAY02 Mass Chromatogram	MRM of 3 Channels AP+
100       Image: Children in the image: Children in	TIC 5.49e3
0.47	Time
0.50 1.00 1.50 2.00 2.50 3.00	3.50
Select mass/wavelength chromatogram	

C. MassLynx 主畫面左側點選 TargetLynx 分頁, 再點選 Edit Method, 出現

Farg	jetLynx 設定視窗		•								
🌱 Ma	ssLynx - Elton - curcumin.SPL										x
<u>F</u> ile	<u>V</u> iew <u>R</u> un <u>H</u> elp										-1
2	- 🗅 🗞 🔒 🎒 🕨		Shortcut	)ueue	🜀 Status						
	Oueue Is Empty										
Ħ	Target you VC	Spec	trum Chromatograr	n Maj	o Edit <del>•</del>	Samples	-				
La L		· ·	File Name	Inlet File	MS File	MS Tune File	Bottle	Inject Volume	Sample Type	Conc A	Qua 🔺
1 ž		383	0923_SC_05ppb_2	0912	CUR+COG	0909 curcu	1:B,2	2.000	Standard	0.5	1
lis		384	0923_Mock+Sd_05ppb_3	0912	CUR+COG	0909 curcu	1:B,4	2.000	Analyte		
	Edit Method	385						0.000			
ő		386						0.000			
Ĕ		387						0.000			
ž		388						0.000			
۲ ۲	Process Samples	389						0.000			
per	(PR)	390	0923_TEST					0.000			
		391						0.000			
N N N	Manu Basulta	392	0920_mix_500ppb_MRM_2	0912	CUR+COG	0909 curcu	1:B,2	2.000	Standard	100ppb	
ž	VIEW Results	393	0920_no inject_4	0912	CUR+COG	0909 curcu	1:C,1	2.000			
Ē.	0	394	0920_mix_500ppb_MRM	0912	CUR+COG	0909 curcu	1:B,2	2.000	Standard	100ppb	
ge		395	0920_no inject_1	0912	CUR+COG	0909 curcu	1:C,1	2.000			
Tar	TrendPlot	396						0.000			
	•	397	Mock+MeOH_new_3	0912	CUR+COG	0909 curcu	1:8,4	2.000	Analyte		
	V U	398	Sd_U5ppb_new_3	0912	CUR+CUG	0909 curcu	1:8,5	2.000	Standard	USppb	
ť	System Status	399	Mock+Sd_U5ppb_new_3	0912	CUR+CUG	0909 curcu	1:8,6	2.000	Analyte		
Ste	-,	400	Mock+Sd_U5ppb_new_2	0912	CUR+LUG	0909 curcu	1:8,6	2.000	Analyte	05h	
ell.	🔴 Not Ready	401	Sa_Uoppb_new_3	0912	CUR+CUG	0909 curcu	1.0.5	2.000	Standard	USPPD OF	
II	(A)	402	Sd_USppD_new_2	0912	CUR+CUG	0909 curcu	1.8,9 1.0 F	2.000	Standard Standard	05ppb	
	Instrument in standby	403	ag_oophp_uew	0312	con+cou	osos curcu	Г. <b>Б</b> ,О	2.000	Stanuaru	ooppo	
l		4									<b>F</b>
Ready				No	ot Scanning		0:0	Only	/ Batch Shutdo	own Enabled	1

 $\overline{\Lambda}$ 

D. 點選 \* 按鈕,新增一項成分數據處理指令。

道 Untitled - TargetLynx XS Method Edit	or							
File Edit Update View Compound	d Help							
🗋 🗳 🔒 🌗 🧇 💠 🗸 😡	🛷 🗞 🔲 📖							
Compound List								
1: New Compound	User Defined Properties	Value	1					
	Compound Name	New Compound						
	CAS Number							
	Compound Type	E						
	Acquisition Function Number	0						
	Quantification Trace							
	Use absolute mass window?	V YES	-1					
	Chromatogram mass window (Da)	0.0200						
	Lecate Beak Using	Potentian Time						
	Locate Peak Osling	Negreet						
	Predicted Retention Time	0.0000						
	Retention Time Window (mins) IO	0.2000						
	Relative Retention Time Reference	None						
	Response Uses	Area						
	Response Type	External (absolute - no internal standards)						
	7.1.0							
	Iotals Group							
	Multiply Traces?	× NO						
	Update Method Times Using Multiple Samples?	NO .	-					
Parala	· · · · · · · · · · · · · · · · · · ·	+ 						
Keady		CAP NUM	11					



E. 點選 Update,勾選定量離子對 Quantitation Ion 以及成分名稱 Compound

#### Name •

표 Untitled - TargetLynx XS Method Edit	or			
File Edit Update View Compound	d Help			
📄 🚅 🛛 🗸 Quantitation Ion	Ctrl+Q			
Compound Noise Range	Ctrl+E			
1: New Co	Ctrl+1		Value	
Second Target Ion	Ctrl+2	and Name	New Compound	
Third Target Ion	Ctrl+3		New Compound	
Fourth Target Ion	Ctrl+4	umber		
✓ Compound Name	Ctrl+M	ind Type	:	Ξ
	Acquis	ition Function Number	0	
	Quanti	fication Trace		
	Use at	osolute mass window?	VES -	1
	Chrom	atogram mass window (Da)	0.0200	
	Landa	Deskiller	Determine Time	
	Locate	Peak Using	Retention Time	
	Dredic	ted Retention Time	0.0000	
	Retent	ion Time Window (mins) IO	0.2000	
	Relativ	e Retention Time Reference	None	
	Respo	nse Uses	Area	
	Respo	nse Type	External (absolute - no internal standards)	
	Totals	Group		
		<b>T</b> 0		
	Multip	y Iraces?		
	Update	vietnod Times Using Multiple Samples?		
			CAP NUM	di

F. 在定量離子對的層析圖上,按住滑鼠右鍵,劃過待測物訊號峰。





G. 回到 TargetLynx 設定視窗,勾選 Update 選項中的 First Target Ion, 設定

第一	定性	離子	對	0
----	----	----	---	---

A Untitled	d - Tar	getLynx XS Method Edito	r			x			
File Edit	Upc	late View Compound	Help						
		Quantitation Ion	Ctrl+Q						
Compour		Noise Range	Ctrl+E						
1: nocon	<ul> <li>Image: A set of the set of the</li></ul>	First Target Ion	Ctrl+1		M-Lu-				
1. Hocon		Second Target Ion	Ctrl+2	red Properties	Value				
		Third Target Ion	Ctrl+3	Ind Name	nocompound				
		Fourth Target Ion	Ctrl+4	imber					
		Compound Name	Ctrl+M	und Type		E			
			Acquis	ition Function Number	1				
			Quanti	fication Trace	294.1 > 64				
			Use at	osolute mass window?	VES YES				
			Chrom	atogram mass window (Da)	0.0200				
				8.1.1.1					
			Locate	Peak Using	Retention Time				
			Locate	Peak Selection	Nearest				
			Predic	ted Retention Time	2.8250				
			Retent	Ion Time Window (mins) IO	0.2450	_			
			Relativ	e Retention Time Reference	None				
			Respo	nse Uses	Area				
			Respo	nse Type	External (absolute - no internal standards)				
			Totals	Group					
			Multipl	y Traces?	× NO				
			Undate ∢	Method Times Using Multiple Samples?		-			
		]			CAP N	NUM			

H. 在第一定性離子對的層析圖上,按住滑鼠右鍵,劃過待測物訊號峰。重複步



驟 C~H,將每個待測物成分都建立定量分析指令。

I. 重複步驟 C~H,將每個待測物成分都建立定量分析指令。

J. 詳細 TargetLynx 設定說明,請參考附錄二、TargetLynx 設定說明。

#### 2. 數據處理

A. 樣品清單選擇數據,點選 TargetLynx 分頁,再點選 Process Samples。

Ma	assLynx - Quantify - Quantify.spl											
Eile	<u>File View Run H</u> elp											
2	🕰 🗸 🗅 🖹 📕 🦾 🖒 🔲 🛄 🖉 Shortcut											
	Queue 1s Empty											
at a	TargetLynx XS 🕖	Spec	trum Chro	matogram	Map Edit -	Samples -		<b>B</b>				
Ě			File Name	Sample ID	File Lext	MS File	Inlet File	Bottle	Inject Volume   Sample A			
str		1	ASSAYU1		plasma blank	DEFAULT	DEFAULT	1	10.000 Blank			
5	G	2	ASSAYU2	102	U.2pg/ml std			2	10,000 Standard			
<u>v</u>	Edit Method	3	ASSATU3	103	0.5pg/mista			3	10.000 Standard			
<u></u>		4	ASSATU4		0.75pg/mista			4	10.000 Standard			
		5	ASSATUS	IDS	ipg/mista 2pg/mista			о С	10.000 Standard			
ŝ	Process Samples	7	A33A106		5pg/mistd			7	10.000 Standard			
L L	Process Samples	8	ASSATO7		10pg/mistd			8	10.000 Standard			
ð		9	4554700 4554709		15pg/ml/std			9	10.000 Standard			
10		10	ASSAY10	1010	0.3pg/ml.QC			10	10.000 BC			
×	View Results	11	ASSAY11	ID11	2pg/ml.QC			11	10.000 QC			
ŝ		12	ASSAY12	ID12	12pg/mlQC	DEFAULT	DEFAULT	12	10.000 QC			
et		13	ASSAY13	ID13	Rat sample 01	DEFAULT	DEFAULT	13	10.000 Blank			
arg		14	ASSAY14	ID14	Rat sample 02	DEFAULT	DEFAULT	14	10.000 Analyte			
⊢	TrendPlot	15	ASSAY15	ID15	Rat sample 03	DEFAULT	DEFAULT	15	10.000 Analyte			
	$\mathbf{O}$	16	ASSAY16	ID16	Rat sample 04	DEFAULT	DEFAULT	16	10.000 Analyte			
<b>.</b>		17	ASSAY17	ID17	Rat sample 05	DEFAULT	DEFAULT	17	10.000 Analyte			
tar	System Status	18	ASSAY18	ID18	Rat sample 06	DEFAULT	DEFAULT	18	10.000 Analyte			
ll S	Not Ready	19	ASSAY19	ID19	Rat sample 07	DEFAULT	DEFAULT	19	10.000 Analyte			
nte	- Hot Ready	20	ASSAY20	ID20	Rat sample 08	DEFAULT	DEFAULT	20	10.000 Analyte			
L L	i Instrument in standby	21	ASSAY21	ID21	Rat sample 09	DEFAULT	DEFAULT	21	10.000 Analyte			
		4	1001000	lin an		DEEAU T	DCCALL T	100				
Ready					Not Scanning		0:0	Only Batch Sh	utdown Enabled 🏼 🍢			

B. 勾選 Update Method Times、Update Ion Ratios、Integrate Samples、

Calibrate Standards、Quantify Samples。Method 選擇要套用的

TargetLynx 方法。按下 OK。出現數據處理結果視窗

Create TargetLynx XS Dataset	X
C:\MassLynx\Quantify.PRC	<u>ן</u>
Operations  POSI±IVE Import  Update Method Times  Update Ion Ratios  Integrate Samples  Calibrate Standards  Quantify Samples  Blank Subtract Print Quantify Reports Export Results to LIMS	Quantify         From Sample       1       To Sample       35         Method:       QmethNew          Curve:       Qmeth1          Printing Report Format           File:           LIMS Export           File:
	OK Cancel

#### 3. 閱覽數據

# A. 點選 <sup>●</sup> ▶ 按鈕,可以切換樣品檔案。或是以下拉選單直接選擇樣品檔案。

😼 TargetLynx XS - untitled *									
File Edit View Display Processing Window									
2 💷 🗸 🛤 🖾 🗖 💷 🕼 🚯 🔽									
e e l				_					
칅		#	Name	Туре					
븸	1	1	ASSAY01	Blank					
	2	2	ASSAY02	Standare					
	3	3	ASSAY03	Standare					
	4	4	ASSAY04	Standare					
	5	5	ASSAY05	Standare					
	6	6	ASSAY06	Standare					
	7	7	ASSAY07	Standare					
	8	8	ASSAY08	Standar					
	9	9	ASSAY09	Standar					
	10	10	ASSAY10	QC					
	11	11	ASSAY11	QC					
	12	12	ASSAY12	QC					
	13	13	ASSAY13	Blank					
	14	14	ASSAY14	Analyte					
	15	15	ASSAY15	Analyte					
	- E		•						

ASSAY02 (Standard) ASSAY03 (Standard) ASSAY04 (Standard) ASSAY05 (Standard) ASSAY06 (Standard) ASSAY07 (Standard) ASSAY08 (Standard) ASSAY09 (Standard) ASSAY10 (QC) ASSAY11 (QC) ASSAY12 (QC) ASSAY13 (Blank) ASSAY14 (Analyte) ASSAY15 (Analyte) ASSAY16 (Analyte) ASSAY17 (Analyte) ASSAY18 (Analyte) ASSAY19 (Analyte)

			x
ZA.		1	
Area	ng/ml	S/N	
902	1.22368	293	
852	1.15681	379	
745	1.01116	310	
754	1.02280	313	
716	0.97191	178	
809	1.09819	375	
887	1.20399	493	
821	1.11452	257	
802	1.08881	373	
812	1.10168	188	
1057	1.43433	160	
800	1.08611	299	
971	1.31826	252	
855	1.16048	92	
571	0.77475	272	-

# B. 點選 <sup>◆</sup> <sup>●</sup> 按鈕,可以切換成分。或是可以以下拉選單直接選擇成分。

	Targ	etLy	/nx XS - untitled *							×	
F	ile E	dit	View Display Processing \	Window Help	0						
	26		🛆 🛃   🖾 🗛 🖳 📢	i 🖡 🗸	<	} - [X		L 🗾 🔲 🖸	🔟 🕥 🦪	*   E	3
					I. Std						
					Parent						
Ě		#	Name	Туре	Metabol	ite	Area	ng/ml	S/N		*
빌브	1	1	ASSAY01	Blank			902	1.22368	293		
	2	2	ASSAY02	Standard	1.000	2.79	852	1.15681	379		
	3	3	ASSAY03	Standard	1.000	2.79	745	1.01116	310		
	4	4	ASSAY04	Standard	1.000	2.79	754	1.02280	313		
	5	5	ASSAY05	Standard	1.000	2.79	716	0.97191	178		
	6	6	ASSAY06	Standard	1.000	2.79	809	1.09819	375		
	7	7	ASSAY07	Standard	1.000	2.79	887	1.20399	493		
	8	8	ASSAY08	Standard	1.000	2.81	821	1.11452	257		
	9	9	ASSAY09	Standard	1.000	2.79	802	1.08881	373		
	10	10	ASSAY10	QC	1.000	2.79	812	1.10168	188		
	11	11	ASSAY11	QC	1.000	2.79	1057	1.43433	160		
	12	12	ASSAY12	QC	1.000	2.81	800	1.08611	299		
	13	13	ASSAY13	Blank	1.000	2.82	971	1.31826	252		
	14	14	ASSAY14	Analyte	1.000	2.82	855	1.16048	92		
	15	15	ASSAY15	Analyte	1.000	2.82	571	0.77475	272		-
	•			•			• •			•	

C. 點選 22 按鈕,開啟檢量線視窗,檢示檢量線品質。在檢量線上的標準品點,

#### 按下滑鼠右鍵,選擇 Exclude,可排除標準品點。





A. 點選 ▲ 按鈕,開啟層析圖視窗,檢示層析峰積分品質。滑鼠左鍵點選層析
 峰,再以滑鼠左鍵按住黑色方塊,調整層析峰積分範圍。按下 ▲ 按鈕,寫下
 更改理由,儲存調整積分的結果。

😼 TargetLynx XS - untitled *											
► ■ X XI® \$\\$\\$\\$\\$\\$\\$\\$\\$\\$\\$\\$\\$\\$\\$\\$\\$\\$\\$\											
					COG						
× # Name Ty	pe	Std. Conc	RT	Area	Conc.	S/N	1º Ratio (Actual)	1º Ratio (Pred)	2º Ratio (Actual)	2º Ratio (Pred)	%Dev 🔺
8         8         0923_SC_500ppb_1         St           9         0.01.0HP         0.00000000000000000000000000000000000	andard	500.000	2.94	197241	485.98446	12122	0.435	0.447	1.026	1.004	-2.8
10 10 C1_1HR Ar	nalyte		2.93	809	1.85647	220	0.447	0.447	1.002	1.004	
11 11 C1_2HR_2 Ar	nalyte		2.93	1801	4.30076	466	0.449	0.447	0.942	1.004	
12 12 C1_4HR Ar 13 13 C1_8HR Ar	nalyte nalyte		2.93	4603 3385	8.20362	2349	0.463	0.447	1.061	1.004	
C-libertion 20 Sec 2016 16:20:21								D. Countration			
Compound name: COG			Chron	natogram	Smooth(Mp.2v2)	E2:MDM		No PICS Fit Values C	alculated		
Correlation coefficient: $r = 0.998732$ , $r^{4}2 = 0.9$	97465		0923_30	2_000pp0_1	S11100u1(W11,2X2)	F2.WRW	545.5 > 369.4	No Reference Define	ed		
Response type: External Std, Area			903		COG 2.94	7	4.368e+006	100			
Curve type: Linear, Origin: Exclude, Weighting	g: 1/x, Axis tran:	s: None	04-		213644	⊧¶					
						$\mathbf{A}$					
			-10 +	1			min	%-			
175000			092					1 1			
150000-											
			90	骨鼠之	〒鍵按住	黑色	方塊・調	整積分			m/z
125000-			%								
<u>बि</u> 100000-			-10 -10				min M				
2 TEODO			00000.000	500eeb 1	Omenth(Mar OvO)	CO-HOH	12 sharpele EQ.				
/5000			0923_30	2_200bbp7_1	Sm00un(wm,2x2)	F2.WRW	545.5 > 177				
50000			90 T		COG 2 94	7	4.443e+006	%-			
25000			04		20242	5					
			70			$\Lambda$					
-0 ************************************	300 400	Conc	-10 -10	2 20 2	40 260 280	3 00 3	20 3 40 min	0-4	0 40	0.60 0.80	100
Parete								,	× cos		
											6:20 PM
		2		VV	2				CH E	I 🔺 🚺 📜 🖤	9/29/2016
	Sign	Modifica	ation								
	C	<i>.</i>									
	Ê	🆄 Thiso	peration	may be	signed and/or	r have a	reason for cha	nge.			
		-									
		موال			њ1		_				
		<u>0</u> se		anaiys	151						
		<u>P</u> as	sword:								
		 D					_				
		Don	iain:	JMM27	37		<b>_</b>				
	ΠB	eason for c	hange: -								
		- Select Re	ason -					<u> </u>			
		- Select Re	ason -								
		peak modifi	cation								
	L	Changes m	ade in a	ccordan	ce with SUP 2	345					

#### B. 點選 ≥ 按鈕,可觀看積分過程及紀錄。

	Q	Qu	ıanLynx - Bup	renq	quan01.	qld												_ 6	X		
	Ei	e <u>E</u> c	dit ⊻iew <u>D</u> ispla	ey Pr	rocessing	Security y	<u>V</u> indow	Help						•							
	È		🛆 📩   🖾	Ņ	🍋   🕂	i 🕅 🔹 📫	 * •	+{ }→ ,	X 🛛 🗆	ΙΣ			1 🔒 🔋	?							
										bupren	orphine										
	×		# Name		Туре	Std. Conc	RT	Area	IS Area	Response	Detection Flags	pg/ml	%Dev	Mod.Comment	Mod.User		Mod.Date	Mod.Time	^		
	믝	46	46 bus_cal5_0	46	Standard	280.030	1.81	440.382	2159.715	0.204	MM	298.2	6.5	Peak tailing	MM2777_PF	REECES	08-Dec-04	16:21:14			
		47	47 bus_cal5_0	47	Standard	539.170	1.82	645.461	1867.580	0.346	MM	513.9	-4.7	Peak tailing	MM2777_PF	REECES	08-Dec-04	16:21:45	-		
		40 40 bus_cal5_040 Standard 009.030 1.01 941.321 1000.740 0.330 49 49 bus_cal5_049 Standard 1347.920 1.81 2223.474 2619.078 0.849					MM bb	1280.0	-5.9	Peak talling	MM2///_PF	RECES	U8-Dec-04	16:22:06	-						
		50 50 bus cal5 050 Standard 1860.130 1.81 2729.669 2383.620 1.14								1.145	bb	1730.9	-6.9								
		51 51 bus_cal5_051 Standard 2480.170 1.81 3418.520 2021.829 1								1.691	bb	2561.4	3.3								
		52	52 bus_cal5_0	152	Standard	3208.050	1.81	4634.233	2078.642	2.229	dd	3381.2	5.4								
		53 53 bus_cal5_053 Standard 3989.840 1.80 5937.676 2289.241 2.5								2.594	bb	3935.7	-1.4						-		
Γ		E	Event	Г			0	Details			Peak Area Comments Date Time					ime		User			
Ī	Peał	k modified Sample:bus_cal5_037, Compound:buprenorphine_IS, RT:1									2145.490 Peak tailing 08-Dec-04 16:25:37						MM27	77_PREE	CES		
Ī	Prei	modification peak Sample:bus_cal5_038, Compound:buprenorphine_IS, RT:1								, RT:1.816	881.041					08-Dec-0	04 16::	26:00			
Ī	Peal	mo	dified	Sar	mple:bus	s_cal5_038	, Comp	ound:buprer	orphine_IS	, RT:1.816	1738.326 Peak tailing 08-Dec-04 16:26:00 N					MM27	77_PREE	CES			
Ī	Prei	nodit	fication peak	Sar	mple:bus	s_cal5_038	, Comp	ound:buprer	orphine, R	T:1.823	2645.505					08-Dec-0	04 16::	26:00			_
Ī	Peał	mo	dified	Sar	mple:bus	s cal5 038	, Comp	ound:buprer	orphine, R	T:1.823	4894.830		Pe	eak tailing		08-Dec-0	04 16::	26:00	MM27	77_PREE	CES
ħ	Prei	nodit	fication peak	Sar	mple:bus	s cal5 043	Comp	ound:buprer	orphine IS	. RT:1.806	1595.821					08-Dec-0	04 16::	37:48		_	_
Ī	Peal	mo	dified	Sar	mple:bus	s_cal5_043	, Comp	ound:buprer	orphine_IS	, RT:1.806	2088.415		Pe	eak tailing		08-Dec-0	04 16::	37:48	MM27	77_PREE	CES
ħ	Data	set S	Saved	Sa	ved to 'C	:WassLyn	x\Bupre	enorphine.PF	 O\Buprenc	uan01.qld						08-Dec-0	04 16::	38:36	MM27	77 PREE	CES
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					bupre	norphine		N	IRM of 2 cha	nnels,ES+	Compound na	me: bupre	enorphir	1e 170 - 40 - 0.0	00044						
					1	1.81			41	38.3 > 55.2 260e+005	Calibration cur	ve: 0.0006	- 0.999 657005	* x + 0.00796	585						
	1	00 <sub>3</sub>			22	223.5			1.1	.2000-005	Response type	e: Internal	Std (Re	ef 1 ), Area * (	IS Conc. / IS	S Area )					
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		buprenorphine_IS MRM of 2 channels,ES+					nnels,ES+	<u>ي</u> 2.00						¥.							
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	De	selu.												5	bupreporp	hine			NUM		

C. 點選 国 按鈕 · 開啟 PIC Scan 視窗 · 檢視樣品的子離子掃描質譜圖(下圖)與標

準品碎片質譜圖(Reference Defined)是否相似。





D. 點選 > 按鈕,開啟總表視窗,檢視所有樣品的每一個成分的定量濃度結果。 若有超過品管法規限制的成分,儲存格會標示為紅色。滑鼠指向紅色格子, 可查看超過品質規範的項目。

若檢出濃度低於 Reporting concentration,則會顯示為 Below RL。

若紅色格子中顯示為粗體字,代表檢出濃度超過 maximum concentration。

N	TargetLynx XS - Overview Flagging											
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×	·	Methamidop	Methomyl	Acephate	Atrazine-de	Simazine	Chlortoluron	Monolinuron	Atrazine	Metoxuron	Terbuthylaz	Sebuthylazi
믜	050617_egg_002	Below RL	Below Fil.		Below RL	Below RL	Below RL	Below RL		Below RL	Below RL	Below RL
	050617_egg_003	4.7	4.6	4.2	4.4	4.4	4.6	4.3	4.4	4.5	4.4	4.4
	050617_egg_004	10.5	10.3	10.9	10.3	10.4	10.2	10.4	10.3	10.3	10.1	10.1
	050617_egg_005	25.2	24.9	27.2	25.6	25.5	24.7	25.7	25.2	25.0	24.9	25.1
	050617_egg_006	49.1	50.8	53.5	49.3	49.2	48.9	49.7	50.4	50.4	49.2	49.4
050617_egg_007 75.0 75.2 79.5 74.3 75.8 74.1 75.4 76.5 74.2										74.2	74.4	74.2
	050617_egg_009 Below RL											
	050617_egg_011 050617_egg_007 5 10.5 10.7 10.6 10.5 10.5 10.8 10.6											
	050617 egg 012 2 Methamidophos 8 25.6 25.7 25.4 25.6 25.5 26.0 26.4											26.4
	050617_egg_013	1º Target	Ion Ratio Flag	ged	9	51.1	50.2	49.9	49.6	50.4	50.6	50.2
	050617_egg_014	7 Ratio Lin	atio = 3.55	02	D	74.3	75.8	75.6	75.5	75.1	76.0	74.9
	050617_egg_015	9 Maximum	concentratio	n exceeded	.1	99.6	100.0	99.3	98.9	100.6	99.7	99.7
	050617_egg_016	E Maximum	Concentratio	on: 50.000 ng/m	ow RL	Below RL	Below RL	Below RL	Below RL	Below RL	Below RL	Below RL
	050617_egg_017	9 Concentra	ation: 74.978 n	ıg/ml	D	98.8	100.2	99.1	100.5	99.0	99.9	99.0
	050617_egg_018	9 Reporting	concentration	n exceeded	7	99.9	100.1	99.7	97.5	99.5	99.0	100.8
	050617_egg_019	B Reporting	Concentratio	n: 3.000 ng/ml	ow RL	Below RL	Below RL	Below RL	Below RL	Below RL	Below RL	Below RL
	050617_egg_020	Concentra	ation: 74.978 n	ıg/ml	ow RL	Below RL	Below RL	Below RL	Below RL	Below RL	Below RL	
	050617_egg_021				ow RL	12	Below RL	Below RL	Below RL	Below RL	Below RL	Below RL
	050617_egg_022	2			5	48.9	48.1	49.8	49.4	49.6	42,3	46.6
5 48.9 48.1 49.8 49.4 49.6 #2.3 46.6												
Cu	ustom Reporting: Select reports to generate NUM											



# V. 列印報告

# 1. 編輯報告格式

A. 在 TargetLynx 視窗,點選 File>Report Format

TargetLynx XS - untitled *															×
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Review Dataset				2.93	1801	4.30076	466		0.449		0.447	0.942	1	.004	
Unaccent Dataset				2.93	4603	11.20572	2349		0.463		0.447	1.061	1	.004	$\square$
ondeept batabetin			_	2.93	3385	8.20362	731		0.470		0.447	1.051	1	.004	
Apply Layout															+
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Import Quan Data		1.47501	5.70773	10.03280	54.01419	103.91715	490.74536	0.23914	1.91951	3.13965	2.32121	3.32315	0.45440	0.94489	1.1768
POSI±IVE Import		1.10923	5.55590	10.26796	55.03651	107.96707	405.90440		1.00047	4.30076	11.20572	0.20362		1.0/3/1	4.0343
Export	+														
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### B. 選擇想要的範本,勾選 enable。在表格上按下滑鼠右鍵,點選 Change

Column Order · 可增加表格其他欄位。

Compounds Report	Samples Repor	t I	Method Report	Tota	ls Report	Audit Report				
Statistics Report S	ample Template Rep	ort O	verview Report	PICS F	Report	Matrix Factor Report				
General Compound	Summary Report	Sample Su	ummary Report	Calibratio	on Report	Experiment Report				
Orientation       Options       Graph Size         Image: Calibration Information       Image: Calibration Information       Image: Calibration Information         Image: Calibration Information       Image: Calibration Information       Image: Calibration Information         Image: Calibration Information       Image: Calibration Information       Image: Calibration Information         Image: Calibration Information       Image: Calibration Information       Image: Calibration Information         Image: Calibration Information       Image: Calibration Information       Image: Calibration Information         Image: Calibration Information       Image: Calibration Information       Image: Calibration Information         Image: Calibration Information       Image: Calibration Information       Image: Calibration Information         Image: Calibration Information       Image: Calibration Information       Image: Calibration Information         Image: Calibration Information       Image: Calibration Information       Image: Calibration Information         Image: Calibration Information       Image: Calibration Information       Image: Calibration Information         Image: Calibration Information       Image: Calibration Information       Image: Calibration Information         Image: Calibration Information       Image: Calibration Information       Image: Calibration Information         Image: Calibration Information										
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Column Format	-			ТС	hange Col	umn Order				
Sort Ascending Sort Descending										

### 2. 輸出報告

A. 在 TargetLynx 視窗,點選 File>Export,選擇 Current Summary 可匯出當 下瀏覽的樣品與成分的定量結果。選擇 Complete Summary 可匯出所有樣品 與成分的定量結果。匯出的表格格式與瀏覽畫面中的表格相同。

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	Review Dataset				2	2.93	1801		4.30076	466		0.449	(	).447	0.942	1	.004	_
	Unaccent Dataset				1	2.93	4603		11.20572	2349		0.463	(	).447	1.061	1	.004	_
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	POSI+IVF Import		1.18923	3 5.	55590	10.2679	8 55.0	3651	107.96707	485.98446		1.85647	4.30076	11.20572	8.20362		1.07371	4.6343
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B. 點選 File>Print,可列印紙本報告。

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	Close					00	G								
	Save	Ctrl+S					<u> </u>								
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	Refresh		a 500.000	2.94	197241	465.96446	12122		0.435		0.447	1.026	1	.004	2.8
	Accept Dataset			2.93	809	1.85647	220		0.447	(	0.447	1.002	1	.004	_
	Review Dataset			2.93	1801	4.30076	466		0.449	(	0.447	0.942	1	.004	$\mp$
	Unaccept Dataset			2.93	4603	11.20572	2349		0.463	(	0.447	1.061	1	004	-
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	Import Quan Data		1.47501 5.70	773 10.0	3280 54.0	1419 103.9171	5 490.74536	0.23914	1.91951	3.13965	2.32121	3.32315	0.45440	0.94489	1.1768
	POSI±IVE Import		1.18923 5.55	590 10.2	6798 55.0	3651 107.9670	485.98446		1.85647	4.30076	11.20572	8.20362		1.07371	4.6343
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# VI.附錄一、儀器方法設定

# 1. Inlet File – 泵浦設定

🚓 ptg_waters4.qsm, ptg_waters4.ftn, ptg_waters4.welsd, ptg_waters4.wpda - Inlet Method										
File View Tools L	File View Tools LC Acquity Sampler Diode Array Help									
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19	Status									
Status	Status ACQUITY Additional Status Solvent Levels									
	☐ Indicators □ Pumps									
	Running 🚺 Time (mins): 0.00	%								
Inlet	Pump On	%								
a la	Flow (ml/min): 0.00	%								
Autosampler	🗧 🗧 Ready									
Autosampier	OK Pressure (psi): -0 👸 100.0	%								
	Detector									
Acquity ELSD Scan: Mode: Idle										
$\mathbf{O}$										
For Help, press F1										

A. ACQUITY UPLC H-Class, 設定四溶媒系統 Quaternary Solvent Manager

Modify A	٩CQ	UITY Quate	ernary Solve	nt Manage	er Instrume	ent Metho	d						×
Acqu	uit PLC*	y Quat	ernary S	Solvent	t Manag	ger	Auto∙Blen Plus™	d Run 1 25	Time:	: min	1		
Gener	al	Misc Dat	ta										
⊏ Sol	vent	s	-			Pressure Limits ?							
Δ	0 1	- 1% FA water	<b>T</b>	1	0								
<u>^</u>				Low:	Ju	psi							
В	B 0.1% FA ACN						15000	psi					
С	0.1	1% FA in Met	thanol 💌										
D			<b>_</b>	No C	hange 🔻	Seal Wa	ash Period:	5.00	mi	n			
	-			Jinore				10.00					
Gradi	ient:												
		Time	Flow (mL/min)	%A	%B	%C	%D	Curve					
1	1	Initial	0.500	100.0	0.0	0.0	0.0	Initial		**			
2	2	10.00	0.500	0.0	100.0	0.0	0.0	6					
3	3	15.00	0.500	0.0	100.0	0.0	0.0	6					
4	4	20.00	0.500	100.0	0.0	0.0	0.0	6	-				
Comn	nent	:											
											_		- 1
										ОК		Cance	

- ✓ Solvent: 可選擇移動相溶劑種類。
- ✓ Flow (mL/min): 輸入移動相流速。
- ✔ Pressure Limits: 最高 15000psi。
- ✓ Gradient
  - Time(min): 輸入梯度變化的時間點。
  - Flow (mL/min): 輸入移動相流速。
  - %A/%B:移動相比例。
- ✓ Run Time: 須大於或等於梯度表最後時間

B. ACQUITY UPLC I-Class, 設定二溶媒系統 Binary Solvent Manager

🗄 Modify Binary Solvent Manager Instrument Method 🛛 🗙											
Binary S	Binary Solvent Manager Run Time: 60.00 min										
General	)ata Anal	og Out   Eve	ents			1					
Solvents	Water Acetonitrile		- 🔟 -	Pressure Low: 0 High: 1	Limits psi 5000 psi	Seal Wash: ? 5.0 min					
Gradient	t			2D Repeat							
	Time (min)	Flow (mL/min)	%A	%В	Curve	+++					
1	Initial	0.400	99.0	1.0	Initial	Gradient Start:					
2	5.00	0.400	99.0	1.0	6	At injection					
3	40.00	0.400	50.0	50.0	6	0.01					
4	40.10	0.400	10.0	90.0	6	Before injection					
5	55.00	0.400	10.0	90.0	6	After injection					
9	55 10	0 400	00 0	10	<u>c</u>	U U					
Comment:											
					(	DK Cancel					

- ✓ Solvent :
  - A1/A2 移動相管路擇一, B1/B2 移動相管路擇一。
  - 可分別註明溶劑種類。
- ✓ Pressure Limits:最高 18000psi。
- ✓ Gradient
  - Time(min): 輸入梯度變化的時間點。
  - Flow (mL/min): 輸入移動相流速。
  - %A/%B:移動相比例。
- ✓ Run Time: 須大於或等於梯度表最後時間



# 2. Inlet File – 自動注射器設定

🚓 ptg_waters4.qsm, ptg_waters4.ftn, ptg_waters4.welsd, ptg_waters4.wpda - Inlet Method								
File View Tools L	File View Tools LC Acquity Sampler Diode Array Help							
🗅 🖻 🖬 🎒 🍊	다   😅 🖬 🚔 🍋 🏣 🌆 🛵 🚜   🛎   🗳							
70	Status							
Status	Status ACQUITY Addition	onal Status   Solvent Levels				_		
	Indicators O Running	Pumps Time (mins):	0.00	Ä	0.0 %			
Inlet	🔵 Pump On	7-		₫	0.0 %			
	<ul> <li>Inject Cycle</li> <li>Ready</li> </ul>	Flow (ml/min):	0.00	6	0.0 %			
Autosampier	🔵 ок	Pressure (psi):	-0	۵	100.0 %			
	Detector Scan:	Mode: Idle						
For Help, press F1								



A. Sample Manager FTN

Modify Sample Manager Instrument Method	×
Sample Manager FTN	Run Time: 1.00 min
General Data Dilution Events	
Solvents	Temperature Control
Wash Solvent Name: 0.1%FA in MeOH	Column:         Alarm Band:           40.0         ▼         □         ±         5.0         ℃
Purge Solvent Name: Water	Sample: Off ▼ ℃ ┌─ ± 5.0 ℃
Pre-Inject Wash: 60 sec	Loop Offline:
Post-Inject Wash: 60 sec	Automatic 🚽 min
	Active Preheater: Use Console Configuration
Comment:	Advanced
	OK Cancel

- ✓ Wash Solvent Name: 選擇 Wash Solvent 溶劑種類。
- ✓ Purge Solvent Name: 選擇 Purge Solvent 溶劑種類。
- ✓ Pre-Inject Wash:抽樣前洗針時間。
- ✓ Post-Inject Wash:注射後洗針時間。
- ✓ Temperature Control
  - Column:外掛 30cm 管柱烘箱時的管柱控制溫度。
  - Sample: 輸入樣品控溫。



B. Sample Manager FL

Modify Sample Manager Instrument Method	×
Sample Manager	Run Time: 1.00 min
General Data Events	
Wash Solvents Weak Wash Name: Strong Wash Name: Weak Wash Volume:	Column:     Alarm Band:       Off     • ℃       Sample:       Off     • ℃       Off     • ℃       ±     5       • ℃     ±       • ℃     ±
Strong Wash Volume:	Disable v min
Max Sample Volume: 0.00 μL Comment:	Advanced
,	OK Cancel

- ✓ Wash Solvent
  - Weak Wash Name:選擇弱洗液溶劑種類。
  - Strong Wash Name:選擇強洗液溶劑種類。
  - Weak Wash Volume: 輸入弱洗液清洗體積。
  - Strong Wash Volume:選擇強洗液清洗體積。
- ✓ Temperature Control
  - Column:外掛 30cm 管柱烘箱時的管柱控制温度。
  - Sample: 輸入樣品控溫。
- ✓ Advanced
  - Injection Mode: 可選擇注射模式, Full Loop、PLNO、Partial Loop。



# 3. Inlet File - 管柱設定

🚓 Untitled.wvhp, Untitled.ftn, Untitled.acm - Inlet Method							
File View Tools L	File View Tools LC Acquity Sampler Help						
🗅   🚔 日   🗁 🗲							
70	Status						
Status	Status ACQUITY Additional Status Solvent Levels						
Status	ndicators Pumps						
	Running     D     Time (mins):     0.00						
Inlet	Pump On     100.0 %						
E Contraction of the second se	Inject Cycle     Flow (ml/min):     0.00     0.0 %						
Autosampler	Ready						
	• OK Pressure (psi): -2 👸 0.0 %						
Acquity CM	Detector Scan: Mode: Idle						
For Help, press F1							



### A. Column Manager

📩 Modify ColumnManager Inst	trument Method	×
Column Manager	<ul> <li>Column Selection Run Time: 1.00</li> <li>Advanced</li> </ul>	min
General Data		1
- Temperature		?
Column:	🔽 Alarm Band:	
Off ▼ °C	± 5.0 °C ☐ Shutdown all columns	
Column Selection		
Valve Position:	Equilibration Time	
Column 1	0.1 min	
External Valve 1:	External Valve 2: External Valve 3:	
No Change 💌	No Change 💌	
Comment:		
	OK Cance	el

- ✓ Temperature
  - Column: 輸入管柱控温。
- ✓ Column Selection :
  - Valve Position:選擇 Column 位置。



### 4. MS File - 質譜儀紀錄模式設定

A. MS Scan 🏼 MS Scan

Function:1 MS Sc	an	
Mass (m/z)		Method
Start	50	Ionization Mode ES+ -
End	650	Data Continuum 👻
Time (Mins)		Scan Duration (secs)
Start	0	Scan Time 0.5
End	5	
Cone Voltage		Probe Temperature
📃 Use Tune P	age	Use Tune Page Settings
Cone Voltage (\	/) 20	Probe Temp 20
🔲 Use Cone V	oltage Ramp	Use Probe Temp Ramp
CV Ra	mp	Probe Temp Ramp
		OK Cancel

- ✓ Mass (m/z) Start/End:指定掃描的 m/z 範圍。
- ✓ Time (Mins) Start/Stop: 層析圖紀錄的時間範圍。
- ✓ Ionization Mode:選擇游離法。(ES,電噴灑游離法;API,大氣壓化學游離法;APPI,
   大氣壓光化學游離法;ASAP,固態氣化化學游離法。)
- ✓ Data: 質譜圖中質量訊號峰的紀錄方式。Centroid, 直條圖; Continuum, 連續波峰圖。
- ✓ Scan Duration(secs): 質譜圖指定之 m/z 範圍的掃描速率。設定值越大, 質譜圖感度越弱, 層析圖點數越多。採用預設值即可。
- ✓ Cone Voltage: 指定進樣錐電壓。或是 Use Tune Page 依照 Tune Page 的進樣錐電壓。
   設定值越大,離子在進樣錐碎裂的機會越大,越不容易發現指定的離子訊號。



Function:1 SIR							
Method		Channels					
Ionization Mod	e ES+ 🔻		Compound Name	Mass (m/z)	Auto Dwel	Dwell (s)	Cone (V)
Span	0	1		]		0.025	
Retention Wir Start End	dow (Mins) 0 16						
Probe Temper	ature	511					
Use Tune Pag	e Settings 🛛 🖳						
Probe Temp	20						
Use Probe Ter	np Ramp			III			
			Delete		Linda	Rodo	Fill Down

- ✓ Ionization Mode:選擇游離法。(ES · 電噴灑游離法; API · 大氣壓化學游離法; APPI · 大氣壓光化學游離法; ASAP · 固態氣化化學游離法。)
- ✓ Span: 允許 m/z 的質量誤差。
- ✓ Retention Window (Mins) Start/Stop: 層析圖紀錄的時間範圍。
- ✓ Compound Name:成分名稱。
- ✓ Mass (m/z):指定 m/z。
- ✓ Dwell (s):四極桿分析 m/z 的維持時間。設定值越大,質譜圖感度越強,層析圖點數越 少。採用預設值即可。
- ✓ Cone Voltage:指定進樣錐電壓。或是 Use Tune 依照 Tune Page 的進樣錐電壓。設定 值越大,離子在進樣錐碎裂的機會越大,越不容易發現指定的離子訊號。



# C. Daughter Scan 🖉 Daughters

Function:1 Daughter Scan	<b></b> X
Mass (m/z) Daughters of 545.50 Start 300.00 End 2000.00	Method Ionization Mode ES+ ▼ Data Continuum ▼
Time (Mins) Start 0 End 16	Scan Duration (secs) Scan Time 1
Collision Energy Use Tune Page Collision Energy (V) 30 Use Collision Energy Ramp CE Ramp	Cone Voltage Use Tune Page Cone Voltage (V) 20 Use Cone Voltage Ramp CV Ramp
Probe Temperature         ✓ Use Tune Page Settings         Probe Temp       20         Use Probe Temp Ramp         Probe Temp Ramp	OK Cancel

- ✓ Daughters of: 指定前驅離子進行碎裂
- ✓ Start/End:指定掃描的m/z範圍。
- ✓ Time Start/Stop (min): 層析圖紀錄的時間範圍。
- ✓ Ionization Mode:選擇游離法。(ES · 電噴灑游離法; API · 大氣壓化學游離法; APPI · 大氣壓光化學游離法; ASAP · 固態氣化化學游離法。)
- ✓ Data:質譜圖中質量訊號峰的紀錄方式。Centroid,直條圖;Continuum,連續波峰圖。
- ✓ Scan Duration(secs): 質譜圖指定之 m/z 範圍的掃描速率。設定值越大, 質譜圖感度越弱, 層析圖點數越多。採用預設值即可。
- ✓ Collision Energy:指定碰撞能量。或是 Use Tune 依照 Tune Page 的碰撞能量。碰撞能量越大碎片越多越小。
- ✓ Cone Voltage:指定進樣錐電壓。或是 Use Tune Page 依照 Tune Page 的進樣錐電壓。
   設定值越大,離子在進樣錐碎裂的機會越大,越不容易發現指定的離子訊號。





Method	Channels									
Ionization Mode ES+ 👻	(	Compound Nam	Parent (m/z)	Daughter (m/z)	Auto Dw	Dwell (s)	Cone (V)	Collision (V)	PIC	Comments
Span 0	1					0.025				
opun										
Use Tune Cone Voltage										
Use Tune Collision Energy										
Betention Window (Mins)										
Chest 0										
Start										
End 16										
Probe Temperature										
✓ Use Tune Page Settings										
Probe Temp 20										
Use Probe Temp Ramp										
Probe Temp Ramp										
PIC Scan										
Use Default PIC Scan function										
PIC Scan Daughter Scan 🔻										
✓ Use Default Threshold										
Activation Threshold 20										
Minimum Threshold 500000										
Use Default Collision Energy										
Collision Energy 20	Add	Delete	Clear All	Undo Re	:do	Fill Down				

- ✓ Ionization Mode:選擇游離法。(ES,電噴灑游離法;API,大氣壓化學游離法;APPI,
   大氣壓光化學游離法;ASAP,固態氣化化學游離法。)
- ✓ Span: 允許 m/z 的質量誤差。
- ✓ Retention Window (Mins) Start/Stop: 層析圖紀錄的時間範圍。
- ✓ Compound Name:成分名稱。
- ✓ Parent (m/z):指定前趨離子 m/z,進行碎裂。
- ✓ Daughter (m/z):指定碎片離子 m/z。
- ✓ Dwell (s):四極桿分析 m/z 的維持時間。設定值越大,質譜圖感度越強,層析圖點數越 少。採用預設值即可。
- ✓ Collision Energy: 指定碰撞能量。或是 Use Tune 依照 Tune Page 的碰撞能量。碰撞能 量越大碎片越多越小。
- ✓ Cone Voltage: 指定進樣錐電壓。或是 Use Tune 依照 Tune Page 的進樣錐電壓。設定 值越大,離子在進樣錐碎裂的機會越大,越不容易發現指定的離子訊號。
- ✓ PIC: 勾選可執行"碎片離子掃描確認"之功能。



# E. Neutral Loss Reutral Loss

Function:1 Neutral Loss	×
Mass (m/z)           Losses of         80.90           Start         300.00           End         2000.00	Method Ionization Mode ES+ ▼ Data Continuum ▼
Time (Mins) Start 0 End 16	Scan Duration (secs) Scan Time 1
Collision Energy Use Tune Page Collision Energy (V) 30	Cone Voltage Use Tune Page Cone Voltage (V) 20
Use Collision Energy Ramp	Use Cone Voltage Ramp
Probe Temperature         ✓ Use Tune Page Settings         Probe Temp       20         Use Probe Temp Ramp         Probe Temp Ramp	OK Cancel

- ✓ Loss of: 指定中性碎片分子量。
- ✓ Start/End:指定掃描的 m/z 範圍。
- ✓ Time Start/Stop (min): 層析圖紀錄的時間範圍。
- ✓ Ionization Mode:選擇游離法。(ES,電噴灑游離法;API,大氣壓化學游離法;APPI,
   大氣壓光化學游離法;ASAP,固態氣化化學游離法。)
- ✓ Data:質譜圖中質量訊號峰的紀錄方式。Centroid,直條圖;Continuum,連續波峰圖。
- ✓ Scan Duration(secs): 質譜圖指定之 m/z 範圍的掃描速率。設定值越大,質譜圖感度越弱,層析圖點數越多。採用預設值即可。
- ✓ Collision Energy: 指定碰撞能量。或是 Use Tune 依照 Tune Page 的碰撞能量。碰撞能 量越大碎片越多越小。
- ✓ Cone Voltage:指定進樣錐電壓。或是 Use Tune Page 依照 Tune Page 的進樣錐電壓。
   設定值越大,離子在進樣錐碎裂的機會越大,越不容易發現指定的離子訊號。



F. Parent Scan 🏼 Parents

Function:1 Parent Scan	×
Mass (m/z)           Parents of         80.90           Start         300.00           End         2000.00	Method Ionization Mode ES+ Data Continuum
Time (Mins) Start 0 End 16	Scan Duration (secs) Scan Time 1
Collision Energy Use Tune Page Collision Energy (V) 30	Cone Voltage Use Tune Page Cone Voltage (V) 20
Use Collision Energy Ramp	Use Cone Voltage Ramp
Probe Temperature         ✓ Use Tune Page Settings         Probe Temp       20         Use Probe Temp Ramp         Probe Temp Ramp	OK Cancel

- ✓ Parents of: 指定碎片離子 m/z。
- ✓ Start/End:指定掃描的 m/z 範圍。
- ✓ Time Start/Stop (min): 層析圖紀錄的時間範圍。
- ✓ Ionization Mode:選擇游離法。(ES,電噴灑游離法;API,大氣壓化學游離法;APPI,
   大氣壓光化學游離法;ASAP,固態氣化化學游離法。)
- ✓ Data:質譜圖中質量訊號峰的紀錄方式。Centroid,直條圖;Continuum,連續波峰圖。
- ✓ Scan Duration(secs): 質譜圖指定之 m/z 範圍的掃描速率。設定值越大,質譜圖感度越弱,層析圖點數越多。採用預設值即可。
- ✓ Collision Energy:指定碰撞能量。或是 Use Tune 依照 Tune Page 的碰撞能量。碰撞能量越大碎片越多越小。
- ✓ Cone Voltage:指定進樣錐電壓。或是 Use Tune Page 依照 Tune Page 的進樣錐電壓。
   設定值越大,離子在進樣錐碎裂的機會越大,越不容易發現指定的離子訊號。

### 5. MS Tune File - 離子化介面設定

Waters Xevo TQ-Smicro MS Detector - D:\test.PRO\ACQU	JDB\20160914_TUVPD	A.ipr				
File View Ion Mode Calibration Gas Vacuum Ran	nps Setup Acquire	Help				
🗋 🚅 🔚 🍜 🛛 📭 🕼 🔯 🔤	> 🗆 11 🛄					
ES- Fluidics Extended Diagnostics			Function	Set	Mass	Span
Source Voltages	_		MS Scan 👻	56	391	500
Capillary (kV) 0.11 2.40		2	MS1 Scan 👻	219	556.3	3
Cone (V) .1 27 -		3	MS1 Scan 👻	502	1121.9	3
Source Temperatures		4	MS1 Scan 👻	614	2017.6	0
Desolvation Temp (*C) 59 350				391.0		8
Cause Cas Flam		1.00e	0			x1
Desolvation (L/Hr)						
Analyser						
HM Resolution 1 14.8						
lon Energy 1						
LM Resolution 2 10.3						
HM Resolution 2 14.9						
lon Energy 2 0.9						
Collision Energy MS (V) 3						
		_	200.0 300.0	400.0	500.0	600.0
<u>"</u>						0
Ready			Vacuu	m Ok	Standby	

- ✓ Capillary (kV):毛細管電壓。
- ✓ Cone (V): 進樣錐電壓。
- ✓ Desolvation Temp(°C):溶媒氣化溫度。
- ✓ Desolvation (L/Hr):毛細管氮氣氣簾流速。
- ✓ Cone (L/Hr):進樣錐氮氣氣簾流速。



# VII. 附錄二、數據處理方法設定

### 1. 層析峰命名設定

A. 在 TargetLynx 設定視窗‧點選 🚰 按鈕

Line TargetLynx XS Method Edito	or .							
File Edit Update View Compound	l Help							
🗋 🗳 🖶 🎒 🍫 💠 🔍	🛷 🔆 🔲 💷							
Compound List								
1: nocompound	Compound Properties	Value						
	Compound Name	nocompound						
	Acquisition Function Number	1						
	Quantification Trace	294.1 > 64						
	Locate Peak Lising	Retention Time						
	Locate Peak Selection	Nearest						
	Predicted Retention Time	2 8250						
	Retention Time Window (mins) IO	0 2450						
	Relative Retention Time Reference	None						
	Response Uses	Area						
	Response Type	External (absolute - no internal standards)						
Ready		CAP NUM						

- ✓ Compound Name: 輸入成分名稱
- ✓ Acquisition Function Number: 對應於 MS File 中的紀錄指令編號
- ✓ Quantification Trace: 定量離子對
- ✓ Locate Peak Using: Retention Time · 以層析峰滯留時間辨識成分
- ✓ Locate Peak Selection: Nearest, 最靠近滞留時間的層析峰才命名
- ✓ Predicted Retention Time: 層析峰預計滯留時間
- ✓ Retention Time Window (mins): 允許的層析峰滯留時間偏移範圍
- ✓ Response Uses: Area · 以面積做為檢量線的 y 軸。
- ✓ Response Type: External · 不含內標準品的檢量線; Internal · 含內標準品的檢量 線。當選擇內標法時,內標準品成分須選擇 External。

#### 2. 檢量線設定

A. 在 TargetLynx 設定視窗,點選 🛂 按鈕

Line - TargetLynx XS Method Edite	or					
File Edit Update View Compound	d Help					
🗋 🗳 🔒 🌗 🧇 💠 🗸 😡	🛷 😽 🔳 🛄					
Compound List						
1: nocompound	Calibration Properties	Value				
	Compound Name	nocompound				
	Calibration Reference Compound	1: nocompound				
	Concentration Units					
	Concentration of Standard: Level	Conc A				
	Stock Concentration Factor	☑ 0.0000				
	Polynomial Type	Linear				
	Calibration Origin	Exclude				
	Weighting Function	1/X				
	Jamese Zees Lawel Otenderde 2	NO.				
	Ignore Zero Level Standards?					
	Ignore Zero Lever QCS?					
	Use Standard Addition?	× NO				
	Propagate Calibration Parameters?	× NO				
Ready	1	CAP NUM				

- ✓ Concentration Units: 濃度單位,例如 ppb。
- ✓ Concentration of Standard Level:標準品或品管標準品的濃度,對應於

樣品清單的濃度欄位。

- ✓ Polynomial Type: Linear · 檢量線為線性模式。
- ✓ Calibration Origin: Exclude · 檢量線不通過原點。
- ✓ Weighting Function: 檢量線加權計算方式 · 1/x 或 1/x<sup>2</sup>。



## 3. 層析峰積分設定

A. 在 TargetLynx 設定視窗 · 點選 🔼 按鈕

🙀 Untitled - TargetLynx XS Method Edit	tor		
File Edit Update View Compoun	d Help		
🗋 🗳 🔒 🌗 🍫 📌 🗸 🗞	🛷 🗞 🔲 🛄		
Compound List	🔒 者 🖾 🎦 🔁 🖳 🖷 省 📲		
1: nocompound	Integration Properties	Value	*
	Compound Name	nocompound	
	Smoothing Enabled?	VES	
	Smooth Parameters		
	Smoothing Method	Mean	
	Smoothing Iterations	1	
	Smoothing Width	2	
	Apex Track Enabled?	× NO	=
	Standard Peak Detection Parameters		-
	Peak-to-peak noise amplitude	✓ 0.0000	
	Balance	0.0000	
	Splitting	0.0000	
	Detect Shoulder Peaks Threshold	₩ 0.0000	
	Reduce Tail	0.0000	
	Reduce Height	0.0000	
	Threshold Parameters		
	Threshold Relative Height	☑ 1.50	
	Threshold Absolute Height	× 0	
	Threshold Relative Area	2.00	
	I hreshold Absolute Area	<b>⋈</b> 0	
	•	m	•
Ready			CAP NUM

✓ 可在 Chromatogram 測試積分後,複製積分方式,在此頁貼上

### 4. 定量與定性離子對設定

A. 在 TargetLynx 設定視窗,點選 💁 按鈕

🕸 Untitled - TargetLynx XS Method Editor			
File Edit Update View Compound Help			
🗋 🚅 🔒 🌗 🧇 💎 🔍	🛷 🗞 🔲 📖		
Compound List			
1: nocompound	Target Ion Properties	Value	
	Compound Name	nocompound	
	Quantification Trace	294.1 > 64	
	Use Quan Ion in Response Calculation?	VES YES	
	Target Ion RT Window (mins) !O	0.3250	
	Target Ion Ratio Method	Quan/Target	
	Calculate Ion Ratio Tolerance As	Ratio	
	Update Ion Ratios Using Multiple Samples?	× NO	
	View First Target Ion Parameters		
	Target Ion Trace	288.1 > 58	
	Use trace in response calculation?	× NO	
	Target Ion Ratio	0.0000	
	Target Ion Ratio Tolerance (%) !O	0	
	Target Ion Must Exist?	× NO	
	Target Ion Must Pass Ratio?	× NO	
	View Second Target Ion Parameters		
	Target Ion Trace		
	Use trace in response calculation?	× NO	
	Target Ion Ratio	0.0000	
	Target Ion Ratio Tolerance (%) !O	0	
	Target Ion Must Exist?	× NO	
	Target Ion Must Pass Ratio?	× NO	
Ready	1	CAP NUM	

- ✓ Quantification Trace: 定量離子對。
- ✓ Target Ion RT Window (min): 定性離子對層析峰的滯留時間的允許誤差範圍。
- ✓ Target Ion Ratio Method: 離子對比值的計算方式。Quan/Target,定量,定性。
   Target/Quan,定性/定量。
- ✓ Update Ion Ratios Using Multiple Samples: 勾選的話・Ion Ratio 期望值來自於・ 樣品清單的 Quan Reference 欄位有 註記的標準品之 Ion Ratio 的平均

土記的標準品之 ION Ratio 的平均

值。

- ✓ Target Ion Ratio: Ion Ratio 期望值。
- ✓ Target Ion Ratio Tolerance (%): 允許樣品中監控成分的 Ion Ratio 的誤差範圍。
- ✓ Target Ion Must Exist: 勾選,才能自動判斷 Ion Ratio 是否超過規格。
- ✓ Target Ion Must Pass Ratio: 勾選,才能自動判斷 Ion Ratio 是否超過規格。



### 5. 法規閾值設定

A. 在 TargetLynx 設定視窗,點選 🎽 按鈕

🎉 Untitled - TargetLynx XS Method Editor			
File Edit Update View Compound Help			
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Compound List	£ ≈ Z A € E ≣ % <mark>1</mark>		
1: New Compound	Sample Flagging Properties	Value	
	Compound Name	New Compound	
	EConcentration Flagging and Reporting Parameters		
	+ Peak Asymmetry		
Ready NUM			

- ✓ Calibration Curve Settings: 檢量線迴歸係數閾值。
- ✓ Signal To Noise Parameters: 訊噪比計算方式,噪音時間範圍設為0,可自動計算。
- ✓ Retention Times Settings: 層析峰滯留時間誤差閾值。
- ✓ Concentration Flagging and Reporting Parameters: 上限濃度(Maximum concentration)與報告濃度(Reporting concentration)閾值。
- ✓ Peak Asymmetry: 層析峰對稱性閾值。