



IDA Information Dependent Acquisition

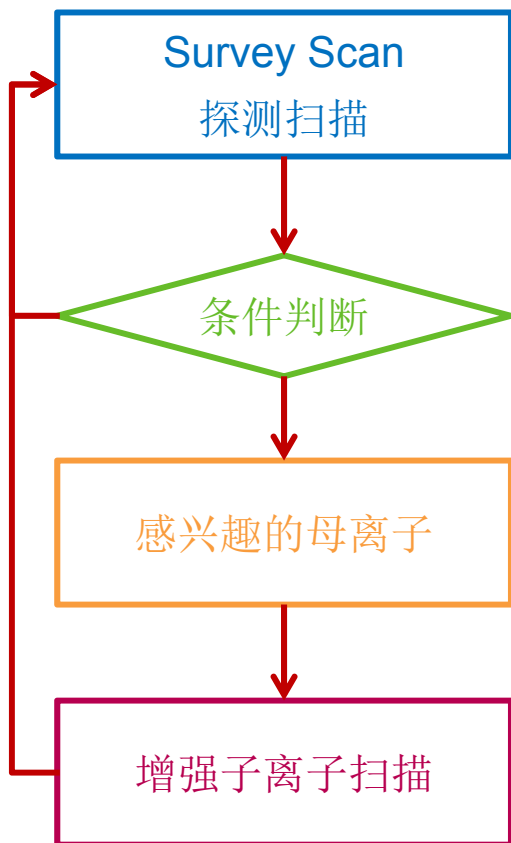
主要内容

IDA工作原理

IDA方法建立

- ✓ 使用IDA Method Wizard
- ✓ 在QqQ方法上扩展

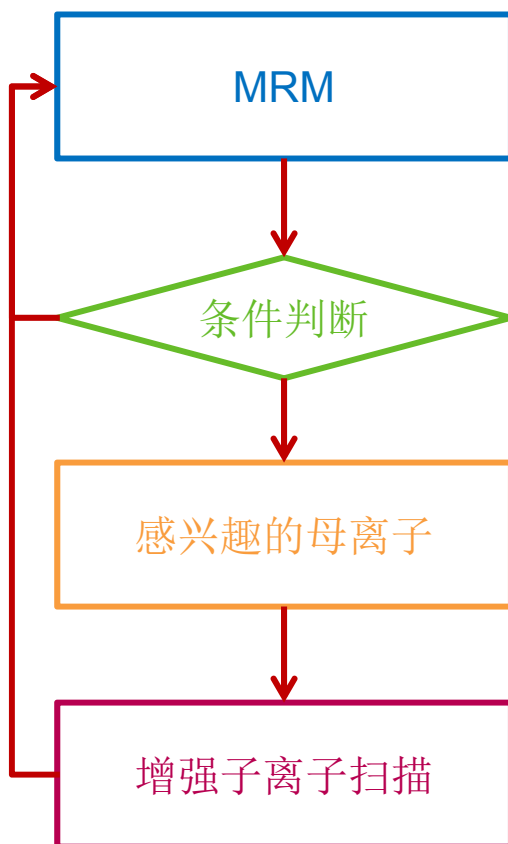
IDA工作原理



- 步骤1，探测扫描
 - 步骤2，系统自动判断：探测扫描采集到的信号强度超过预设值（即“出现色谱峰”）
 - 步骤3，当步骤2的条件满足时，系统自动切换（ $<1\text{ms}$ ）为线性离子阱模式，进行增强子离子扫描（EPI），获得探测扫描所得之母离子的高质量MS2谱图；返回步骤1
- ✓ Survey Scan（探测扫描）可有多种方式，包括MRM、中性丢失扫描母离子扫描等等

IDA基本采样方式

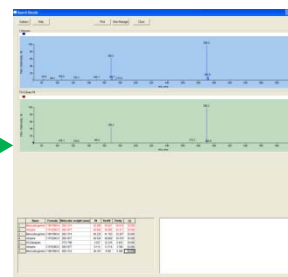
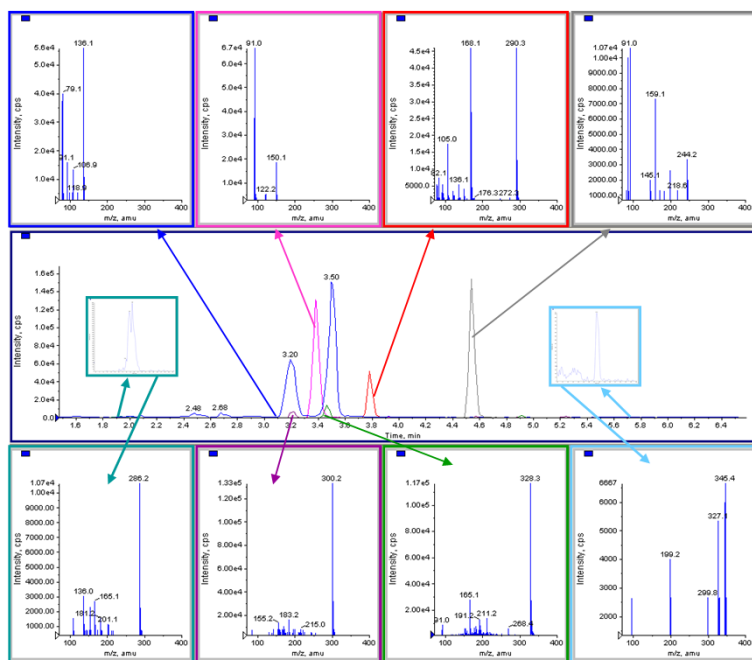
MRM-IDA-EPI



- 以MRM作为探测扫描，触发IDA工作
- MRM列表的获得
 - ✓ 现有的MRM方法
 - ✓ 标准物质方法优化
 - ✓ iMethod™
 - ✓ 通过代谢途径预估 (pMRM)
- 应用于
 - ✓ 农兽药残留定性确证
 - ✓ 阳性确证
 - ✓ 药物代谢产物鉴定
 - ✓ 杂志鉴定
 - ✓

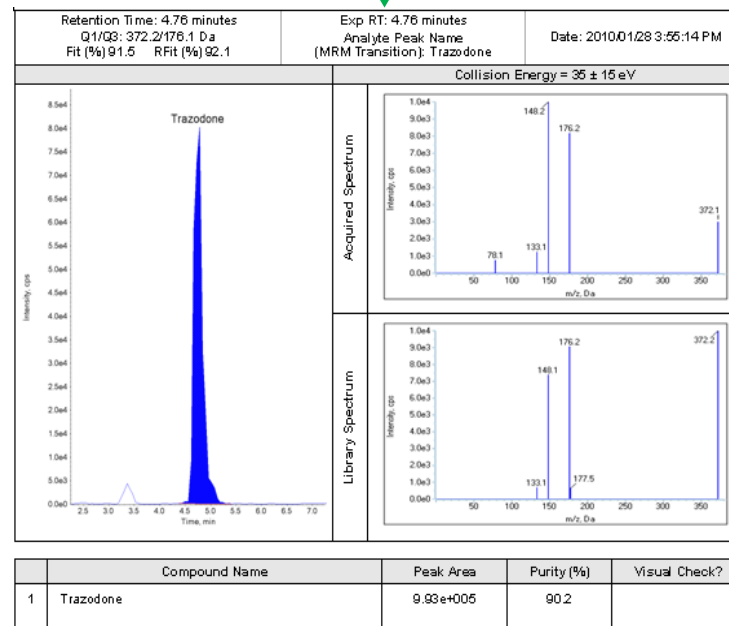
IDA工作流程实例

农兽药残留定性确证



谱库搜索确证

全自动报告



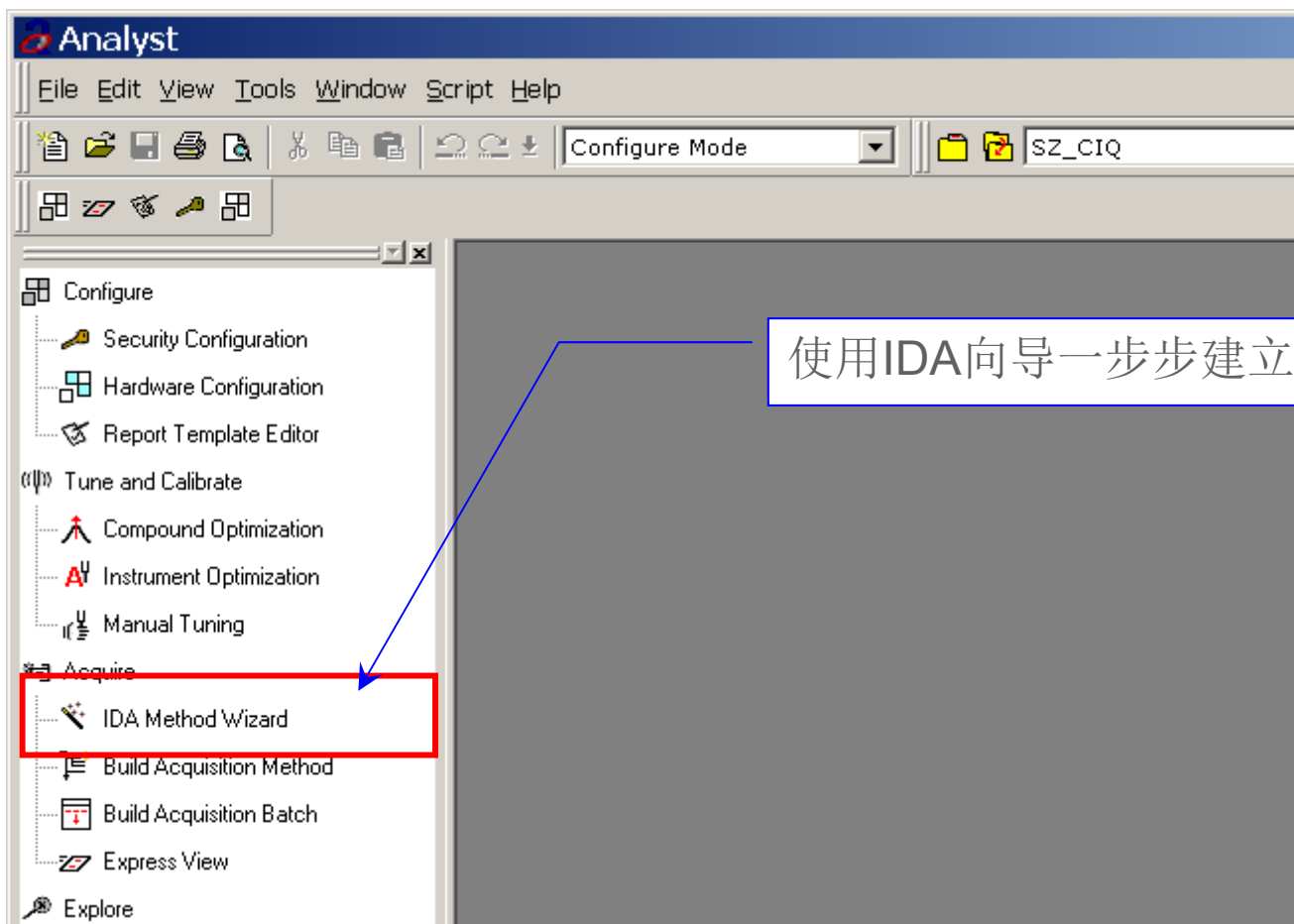
主要内容

IDA工作原理

IDA方法建立

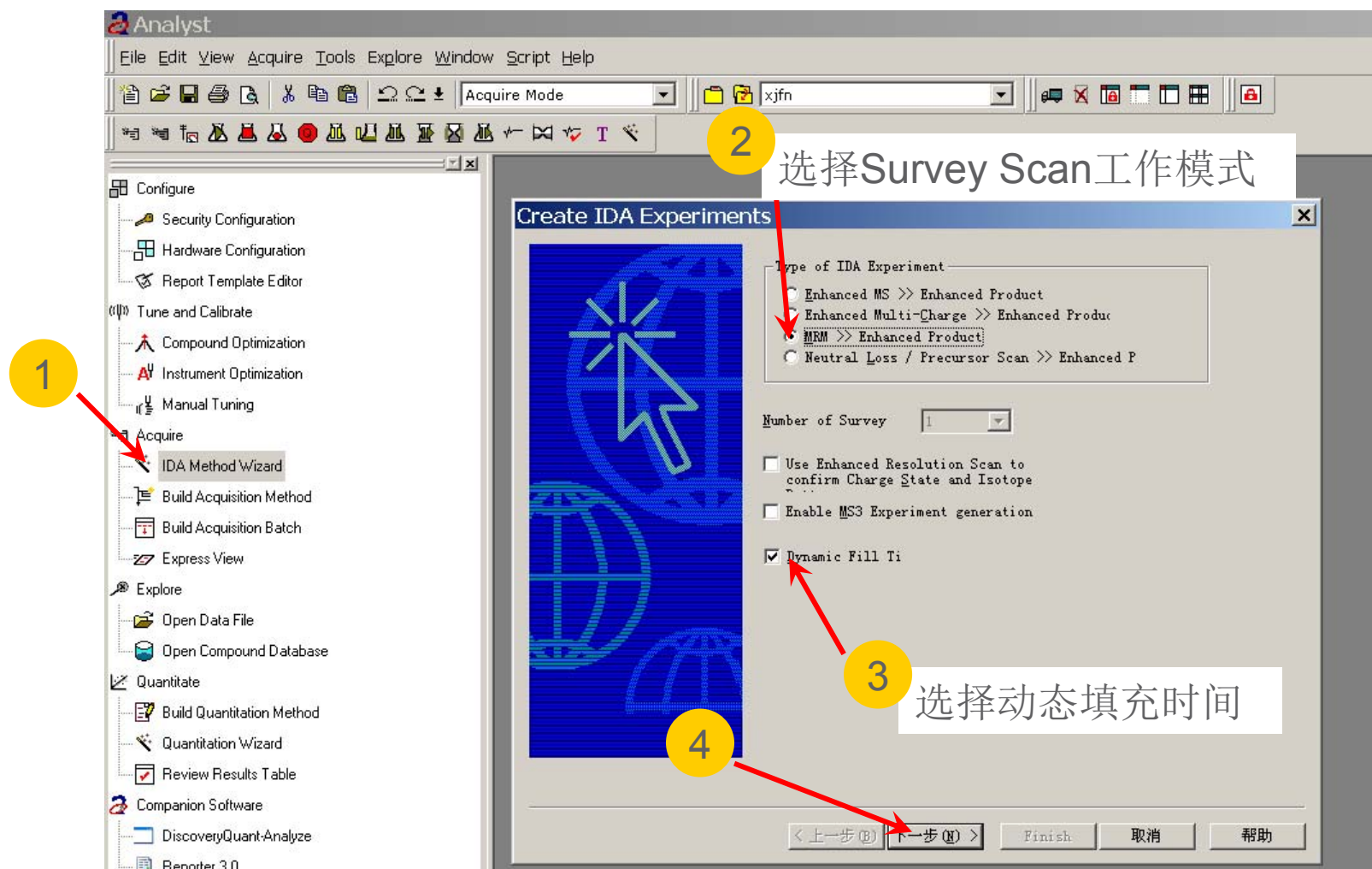
- ✓ 使用IDA Method Wizard
- ✓ 在QqQ方法上扩展

Analyst® 软件使用者界面

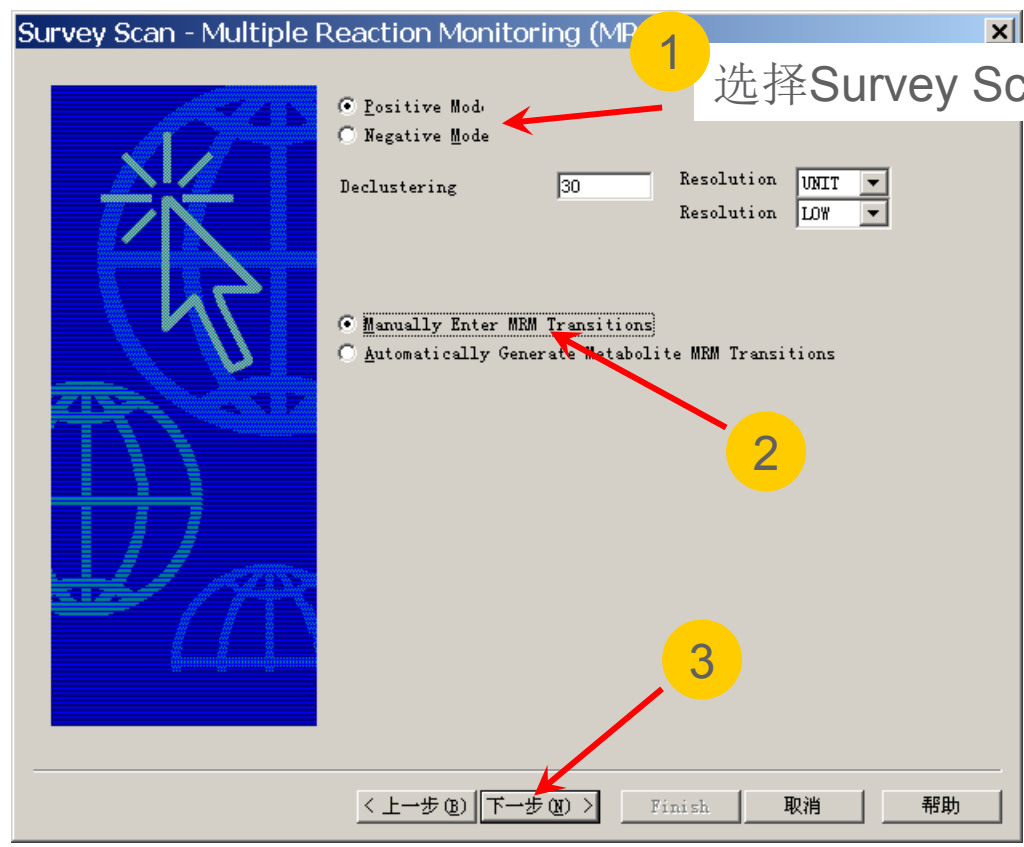


使用IDA向导一步步建立方法

IDA向导，第一步（以MRM触发EPI方法为例）



IDA向导，第二步



选择Survey Scan正负模式

IDA向导，第三步

MRM Transitions

Dwell (ms)

Apply CE to all ! Collision Energy (eV)

	Q1 (Da)	Q3 (Da)	CE (eV)
1	300	100	30
2	200	143	44
3			

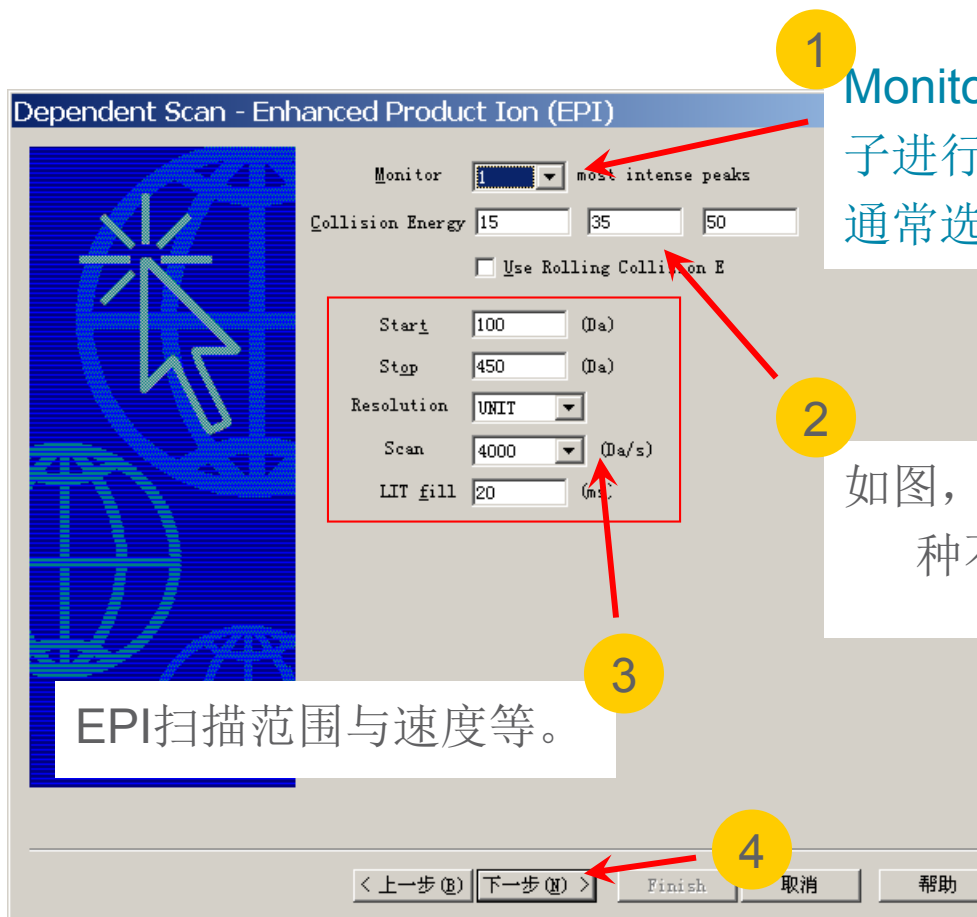
Scan (s)

< 上一步 (P) 下一步 (N) >

1 手工输入MRM列表参数

2

IDA向导，第四步



1 Monitor, 表示每次对最强的X个母离子进行EPI扫描。建议不要超过3个, 通常选1个即可。

2 如图, 同一母离子按照15、35和50三种不同能量得到3个EPI图。

3 EPI扫描范围与速度等。

4

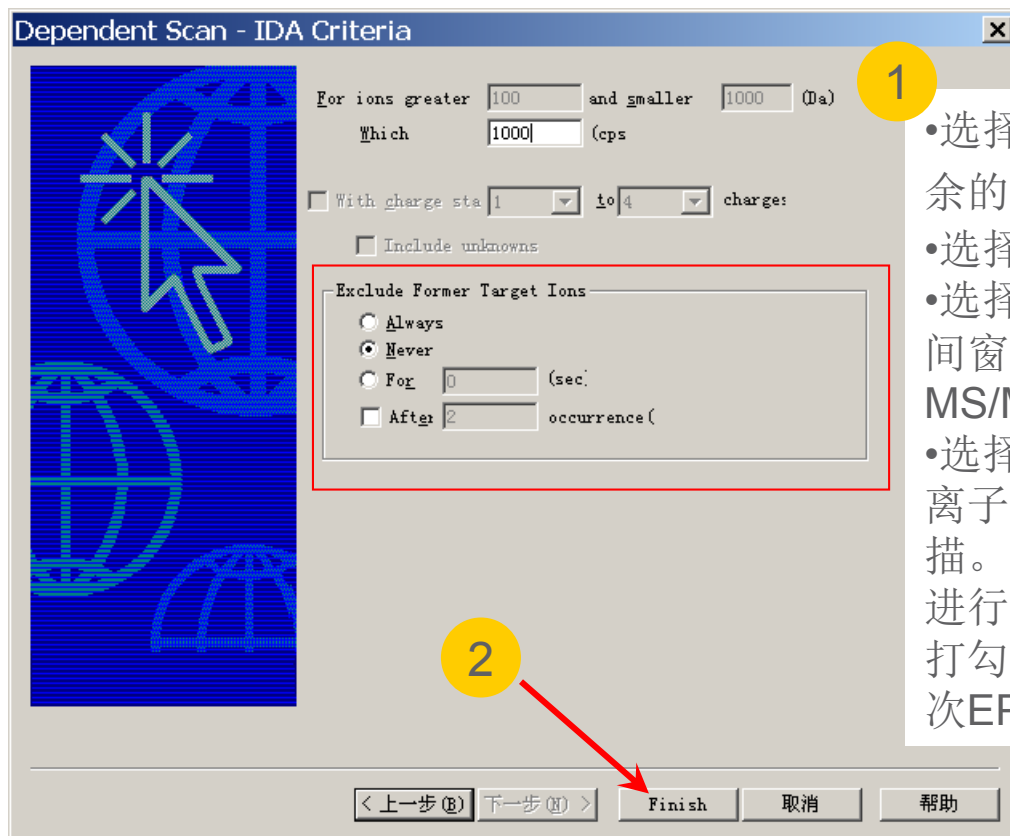
型号	扫描速度 Scan Rate (Da/s)
4500/5500	10000
3200/4000	4000

IDA向导，第五步

1 触发EPI扫描的阈值。一般为数百至数千。

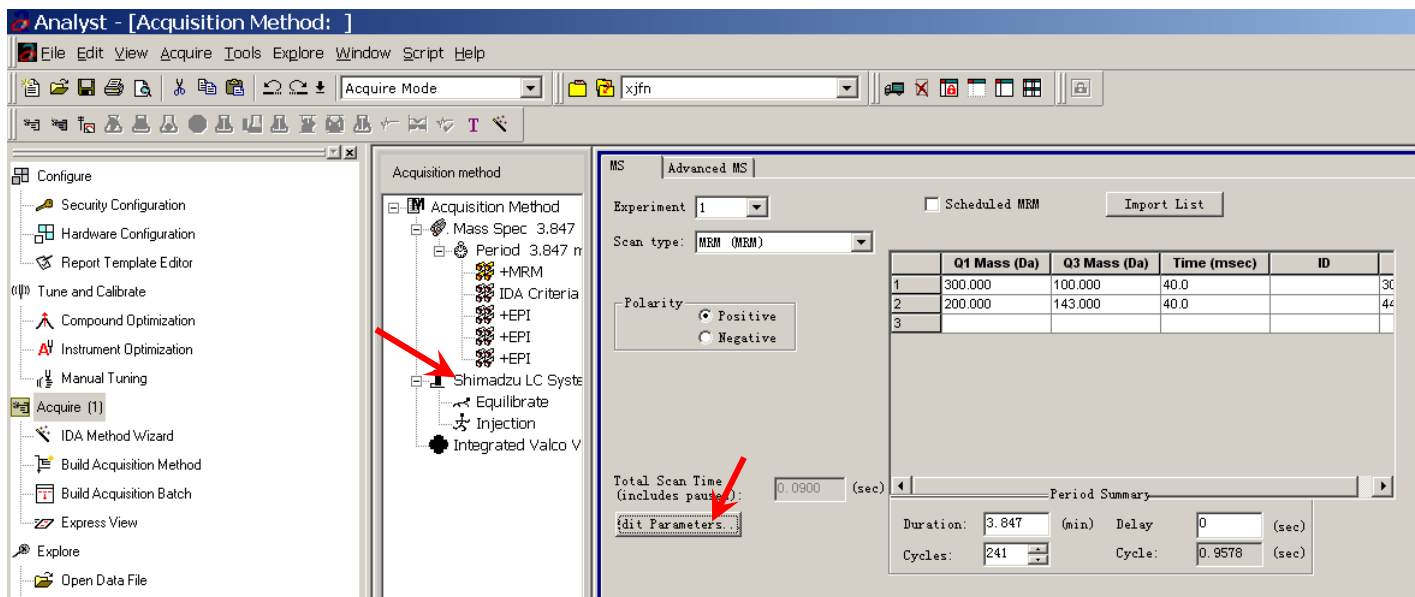
2 是否触发EPI扫描的逻辑条件。

IDA向导，第五步（续）



- 选择Always 可以将这些离子从剩余的运行中排除
- 选择Never打勾，动态排除关闭
- 选择For_(sec)，可以在设定的时间窗口洗脱的母离子不再进行MS/MS扫描
- 选择After_occurrences，允许选择离子在排除之前进行几次MS/MS扫描。此处输入1，则离子在排除之前进行多于一次MS/MS扫描。如果不打勾，则与输入0是一样的，只做一次EPI。

IDA向导，结束



注意：调整离子源参数和液相色谱参数。

主要内容

□ QTRAP工作原理

□ IDA方法原理与使用

✓ 原理

✓ 方法建立的两种途径

在原有QqQ方法基础上直接建立IDA方法 以MRM触发EPI为例

The screenshot shows the 'Advanced MS' configuration window. On the left, a tree view shows the acquisition method structure: Acquisition Method > Mass Spec 19.000 r > Period 19.000 r > +MRM > Shimadzu LC System > Equilibrate > Injection.

The main configuration area includes:

- Experiment: 1
- Scan type: MRM (MRM)
- Polarity: Positive (selected)
- MRM detection: 90 (sec)
- Target Scan Time: 1 (sec)
- Duration: 19.000 (min)
- Delay: 0 (sec)
- Cycles: 1140
- Cycle: 1.0000 (sec)

A table of MRM transitions is displayed:

ID	Q1 Mass (Da)	Q3 Mass (Da)	Time (min)
1	251.200	149.000	3.9
2	251.200	167.100	3.9
3	251.200	191.100	4.1
4	251.200	209.100	3.9
5	251.200	121.100	4.1
6	247.100	189.100	3.3
7	247.100	149.100	3.3
8	307.210	71.000	7.1
9	307.200	167.100	7.3
10	363.200	149.000	8.9
11	363.200	247.100	8.9

在原有QqQ方法基础上直接建立IDA方法 ——第一步

1, 右键点击

The screenshot shows the software interface for configuring an acquisition method. On the left, a tree view shows the acquisition method structure, including 'Mass Spec 19.000 r', 'Shimadzu LC System', 'Equilibrate', and 'Injection'. A red box highlights the '+MEM' icon, and an orange arrow points to it from the text '1, 右键点击'. A context menu is open over this icon, listing the following options:

- Add experiment
- Add IDA Criteria Level
- Copy this experiment
- Delete this experiment

The 'Add IDA Criteria Level' option is highlighted with a red box. In the background, the 'Advanced MS' settings are visible, including a table of MRM transitions:

	Q1 Mass (Da)	Q3 Mass (Da)	Time (min)	ID
1	251.200	149.000	3.9	DPzP 1
2	251.200	167.100	3.9	DPzP 2
3	251.200	191.100	4.1	DPzP 3
4	251.200	209.100	3.9	DPzP 4
5	251.200	121.100	4.1	DPzP 5
6	247.100	189.100	3.3	DAP 1

在原有QqQ方法基础上直接建立IDA方法 ——第二步

Acquisition method

Acquisition Method

- Mass Spec 19.000
- Period 19.000
- +MRM
- IDA Criteria
- Shimadzu LC System
- Equilibrate
- Injection

IDA - First Level Criteria | Include/Exclude | Isotope Pattern

Select: 1 to 1 most intense

After Dynamic Background Subtraction

Survey -> IDA Experiment

- For ions greater 100 (m/z)
- For ions smaller 2800 (m/z)
- With charge sta 2 to 3
- Include unknowns
- Which exceeds: 5000 (cps)
- Rolling Collision E: Settings...

Exclude former target ions

- Always
- Never
- For 0 (sec)

Mass 250 mDa ppm

Exclude isotopes with 4 (Da)

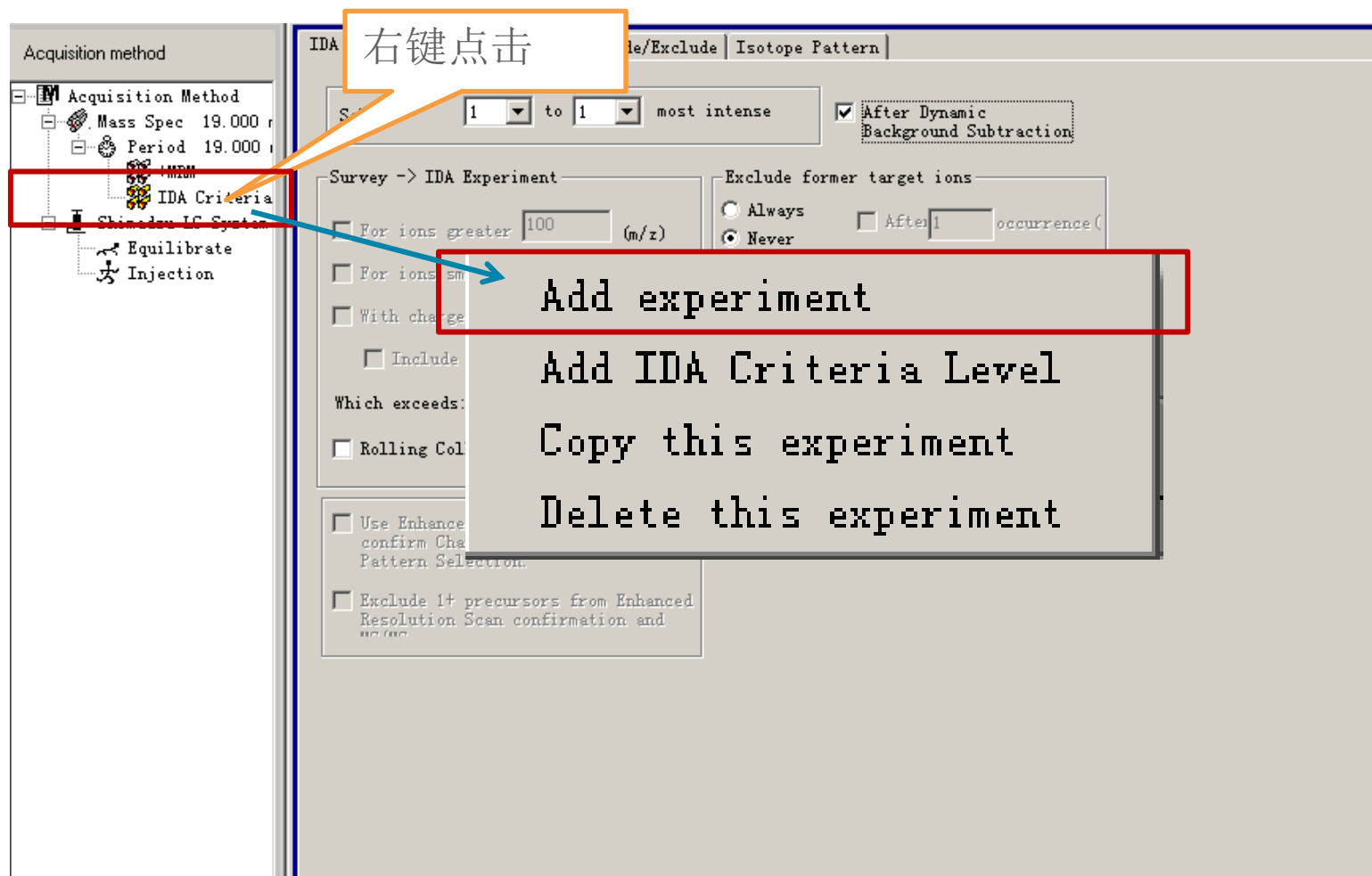
Use Enhanced Resolution Scan to confirm Charge State OR Isotope Pattern Selection.

Exclude 1+ precursors from Enhanced Resolution Scan confirmation and

该选项必选

本页中，绝大多数选项的意义和设定同“IDA向导”。参考32页

在原有QqQ方法基础上直接建立IDA方法 ——第三步



在原有QqQ方法基础上直接建立IDA方法 ——结束

Acquisition method

MS Advanced MS

Experiment: 2

Scan type: Enhanced Product Ion

Scan rate: 4000 (Da/s)

Polarity: Positive Negative

	Start (Da)	Stop (Da)	Time (sec)
1	50.000	70.000	0.0050
2	65.000	137.200	0.0181
3	132.000	400.000	0.0670
4			

MCA

Number of scans to: 1

Product: 30.000 (Da)

Total Scan Time (includes pauses): 0.3906 (sec)

Period Summary

Duration: 19.004 (min) Delay: 0 (sec)

Cycles: 820 Cycle: 1.3906 (sec)

Edit Parameters...

调整离子源参数

注意，调整以下参数：

- Scan rate:
 - 3200/4000: 4000Da/s
 - 4500/5500: 10000Da/s
- Number of scans to: 1

其他注意点

- ❑ 保证Survey Scan（探测扫描）和Dependent Scan（EPI扫描）的离子源参数（Source/Gas）完全一致；
- ❑ 使用IDA方法时，无论Survey Scan（探测扫描）还是Dependent Scan（EPI扫描），CAD（Collision Gas）必须设定为High。
- ❑ IDA 勾选After Dynamic Background Subtraction
- ❑ Exclude former target ions: Never
- ❑ IDA Select 1 to n(EPI数目): 3200&4000 n=1; 5500 n≤3