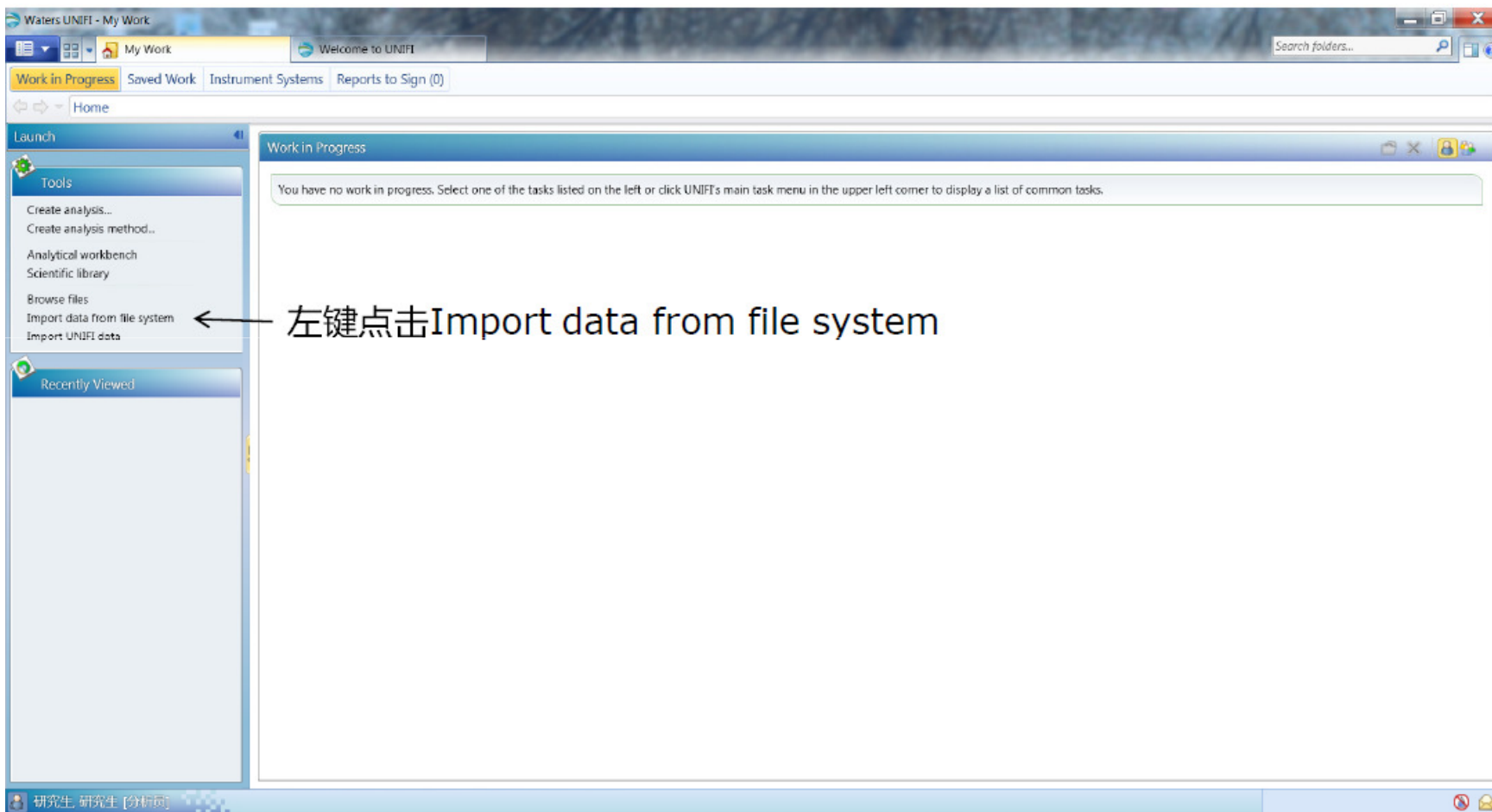


代谢产物鉴定

基本流程

- 导入数据
- 创建分析方法
- 创建分析
- 处理数据
- 浏览结果
- 打印报告

导入masslynx数据



导入masslynx数据

Waters UNIFI - Import File Data

My Work | Welcome to UNIFI | Import File Data

Import File Data

Home

File import settings

Import data type: MassLynx data - Create Sample Set Only

* Group name: Met ID Training

* Group description: 20131231

Selected files

Select File(s)

Select Folders to Import

Company

研究生

310811_036.raw 26.12.2013 5:57 PM

310811_037.raw 26.12.2013 5:57 PM

310811_038.raw 26.12.2013 5:58 PM

310811_039.raw 26.12.2013 5:58 PM

310811_040.raw 26.12.2013 5:58 PM

310811_041.raw 26.12.2013 5:58 PM

310811_042.raw 26.12.2013 5:59 PM

310811_043.raw 26.12.2013 5:59 PM

310811_044.raw 26.12.2013 6:00 PM

Folder: "310811_044.raw" "310811_036.raw" "310811_037.raw" "310811_038.raw" "310811_039.raw" "310811_040.raw" "310811_041.raw" "310811_042.raw" "310811_043.raw" "310811_044.raw"

Select .RAW Folder(s) | Cancel

Import to Folder

3, 左键点击选择输入文件夹位置

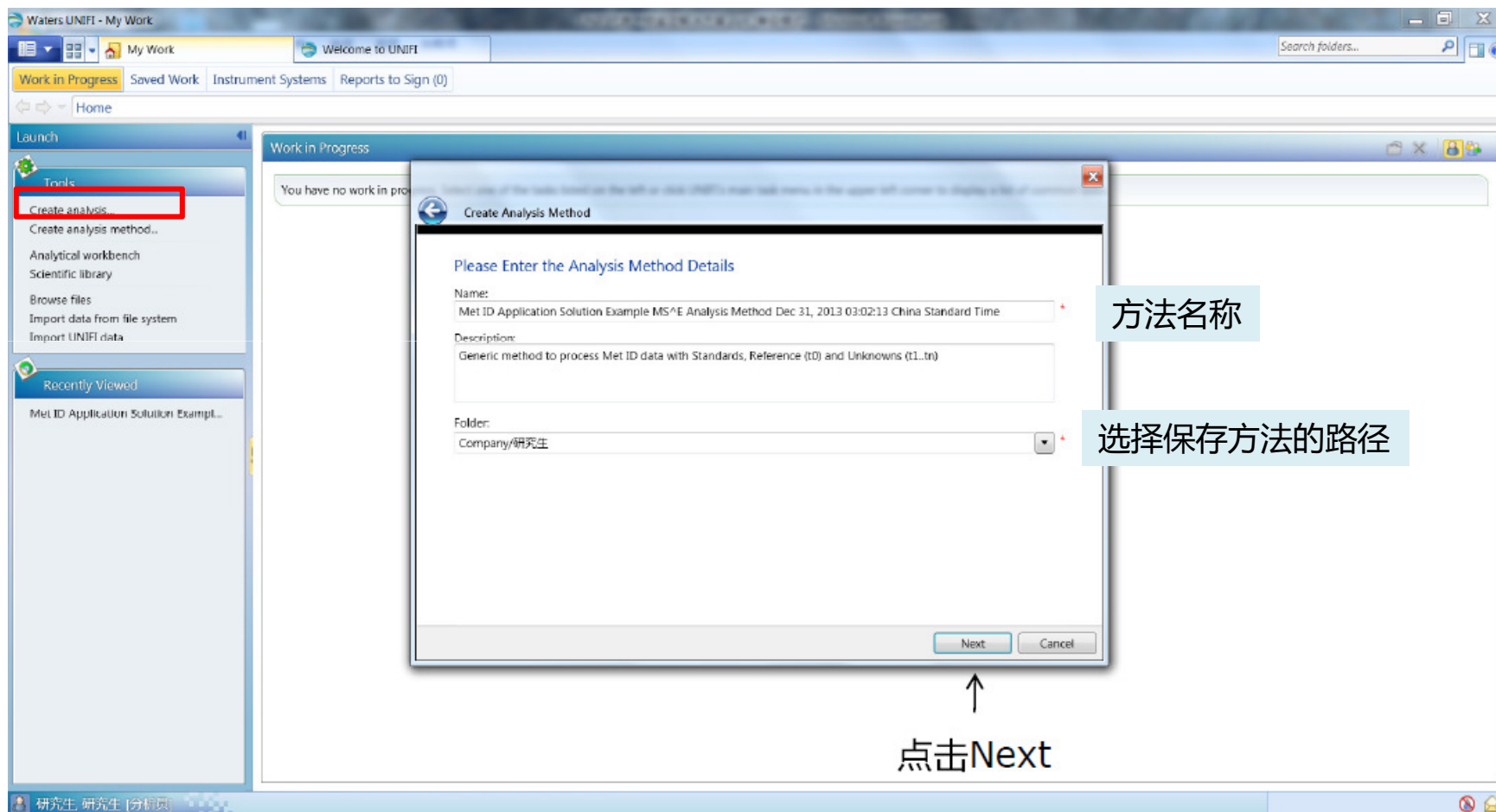
Import

1, 输入 Group name

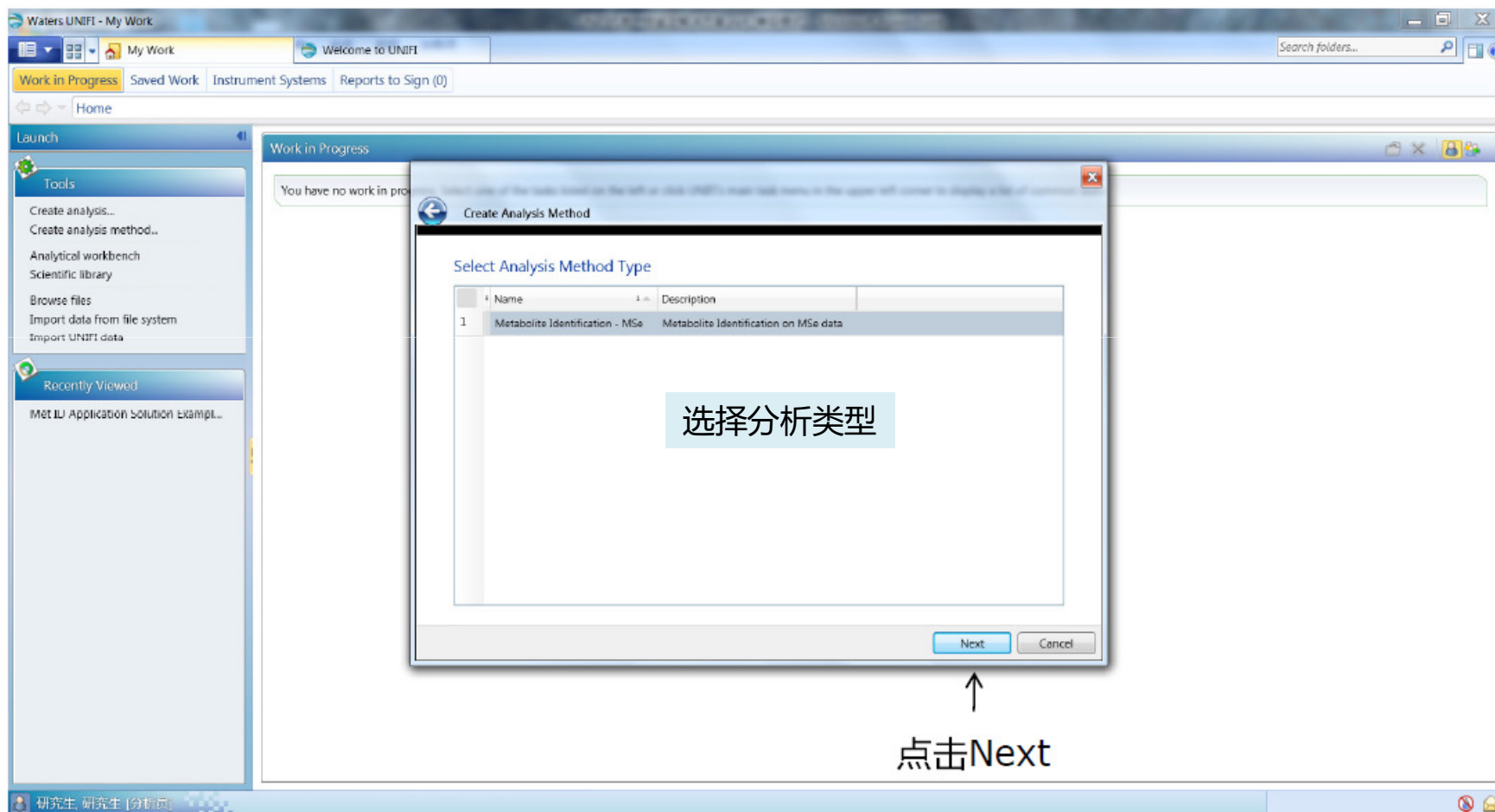
2, 输入 Group description

4, 选择文件所在的文件夹

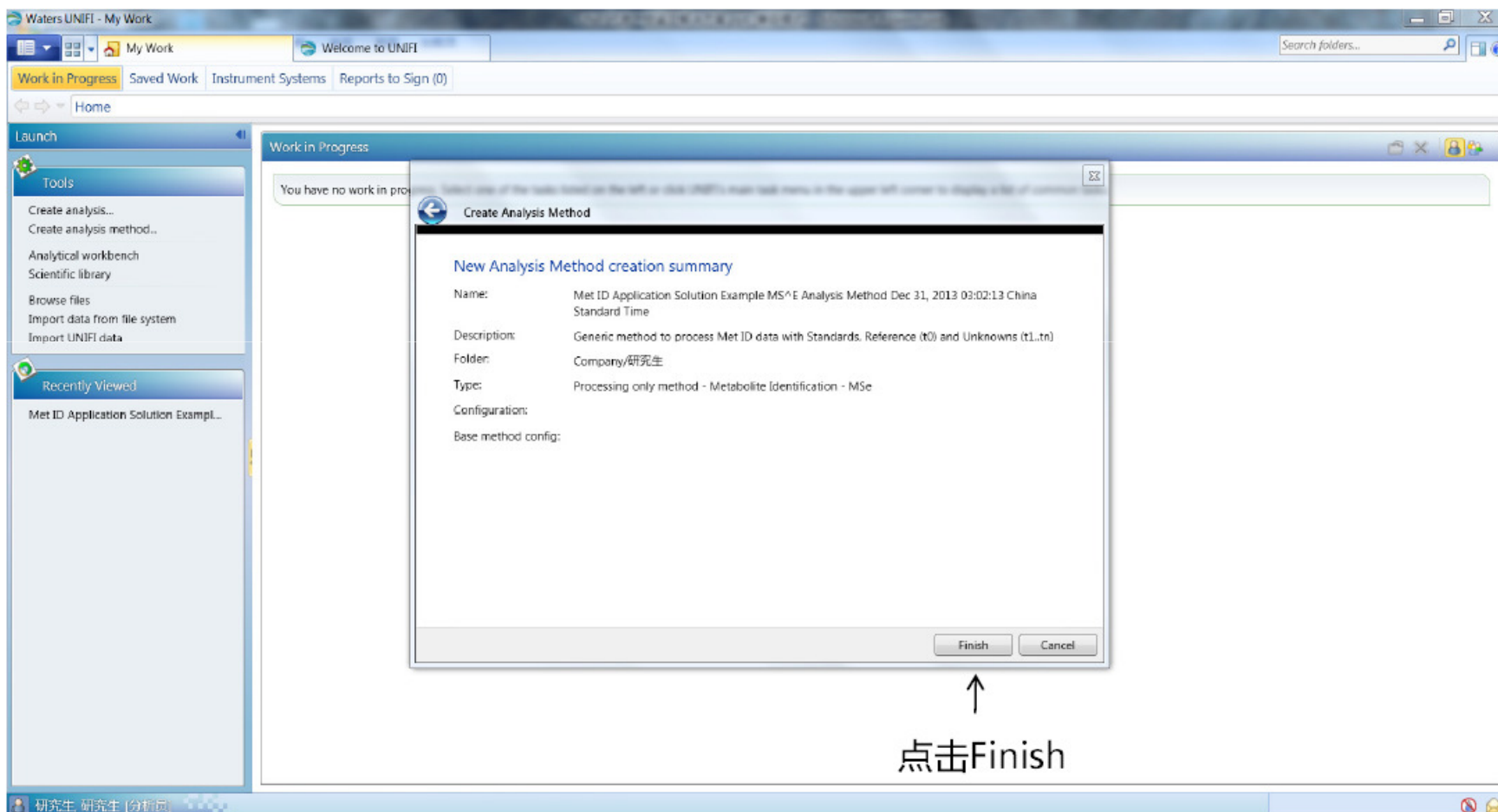
创建分析方法



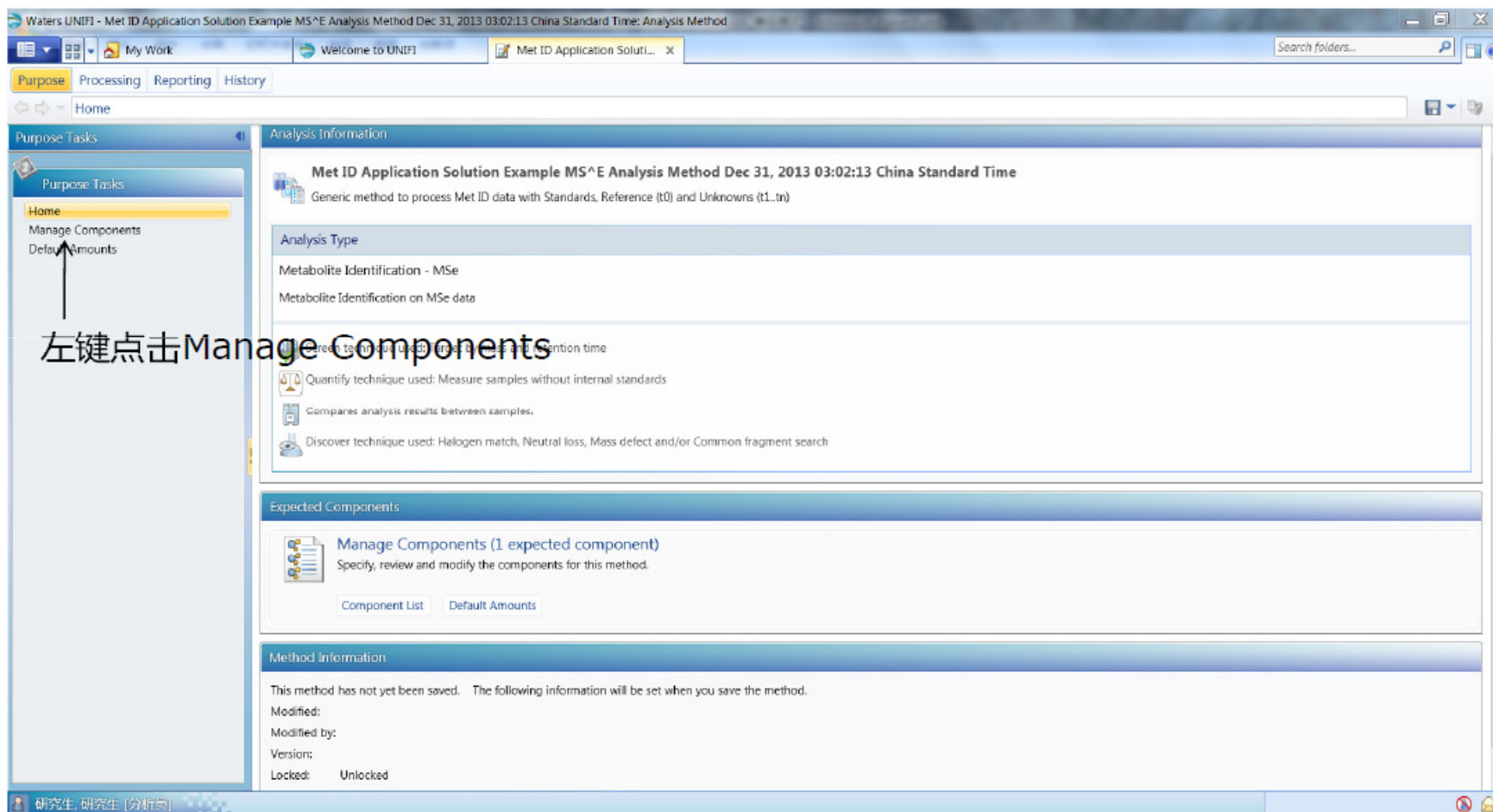
创建分析方法



创建分析方法



编辑原药信息



从数据库导入

1, 左键点击Import

2, 输入药物名称检索数据库

3, 选择数据库

Search criteria

| Search criteria | Operator | Search value |
|-----------------|----------|--------------|
| 1 Name | equals | Nefazodone |

Search in: Amino Acids, Default Custom Library ... Show: 100 Results Search

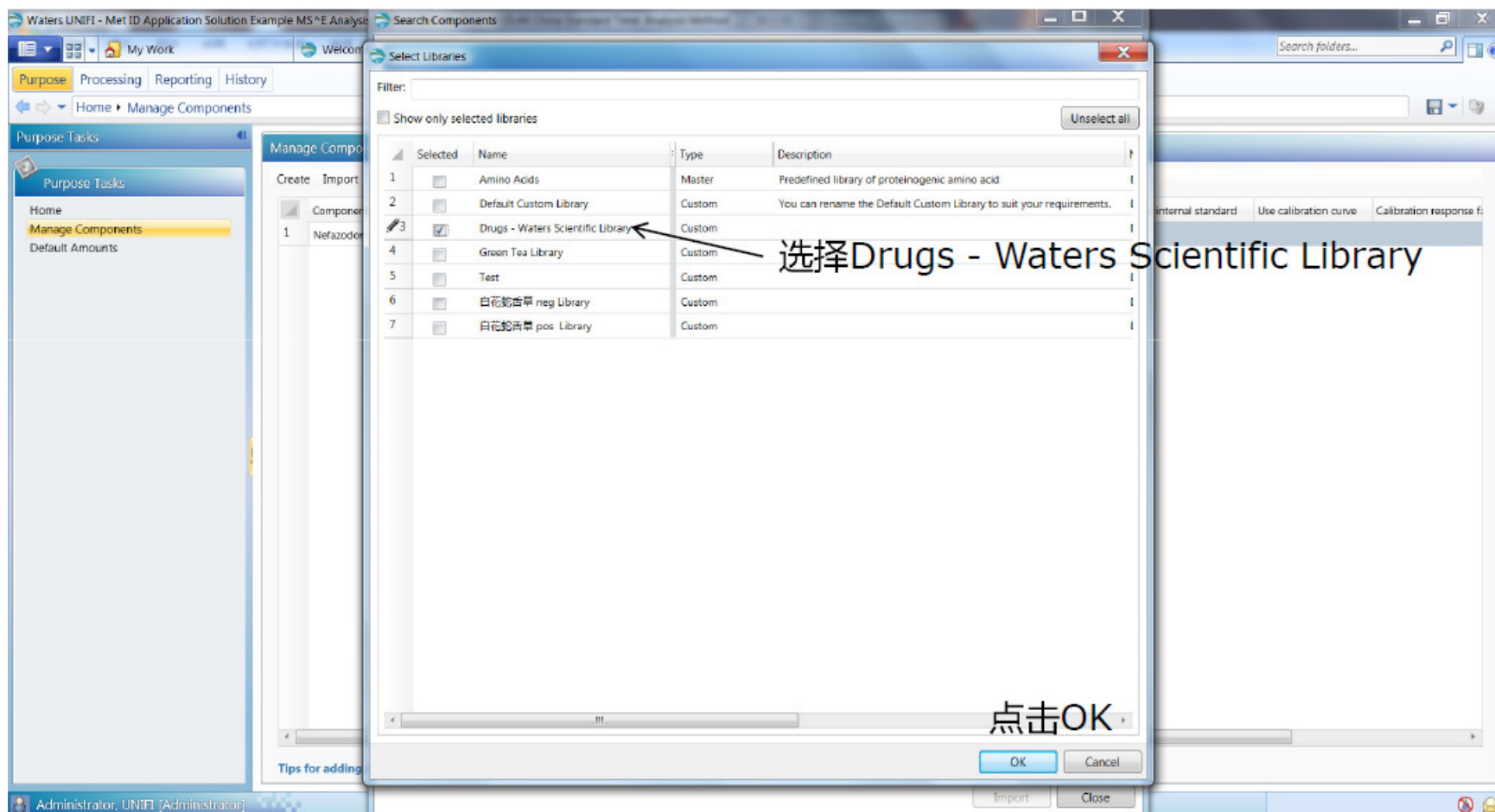
Search R: Select library to search...

Detection results

| Ionization technique | Retention time (min) | Comment | Mass (m/z) | Adduct |
|----------------------|----------------------|---------|------------|--------|
|----------------------|----------------------|---------|------------|--------|

Import Close

从数据库导入



从数据库导入

左键点击Search

| Search criteria | Operator | Search value |
|-----------------|----------|--------------|
| 1 Name | equals | nefazodone |

Search in: Drugs - Waters Scientific Library Show: All Results Search

Search results (1 items found)

| Name | Formula | Has detection results |
|--------------|--------------|--------------------------|
| 1 Nefazodone | C25H32ClN5O2 | <input type="checkbox"/> |

选择结果

Import

Import Close

Waters UNIFI - Met ID Application Solution Example MS^E Analysis Method Dec 31, 2013 19:05:44 China Standard Time: Analysis Method

My Work Welcome to UNIFI Met ID Application Soluti... x Search folders...

Purpose Processing Reporting History

Home Manage Components

Purpose Tasks

Purpose Tasks

Home

Manage Components

Default Amounts

Click Processing

Manage Components

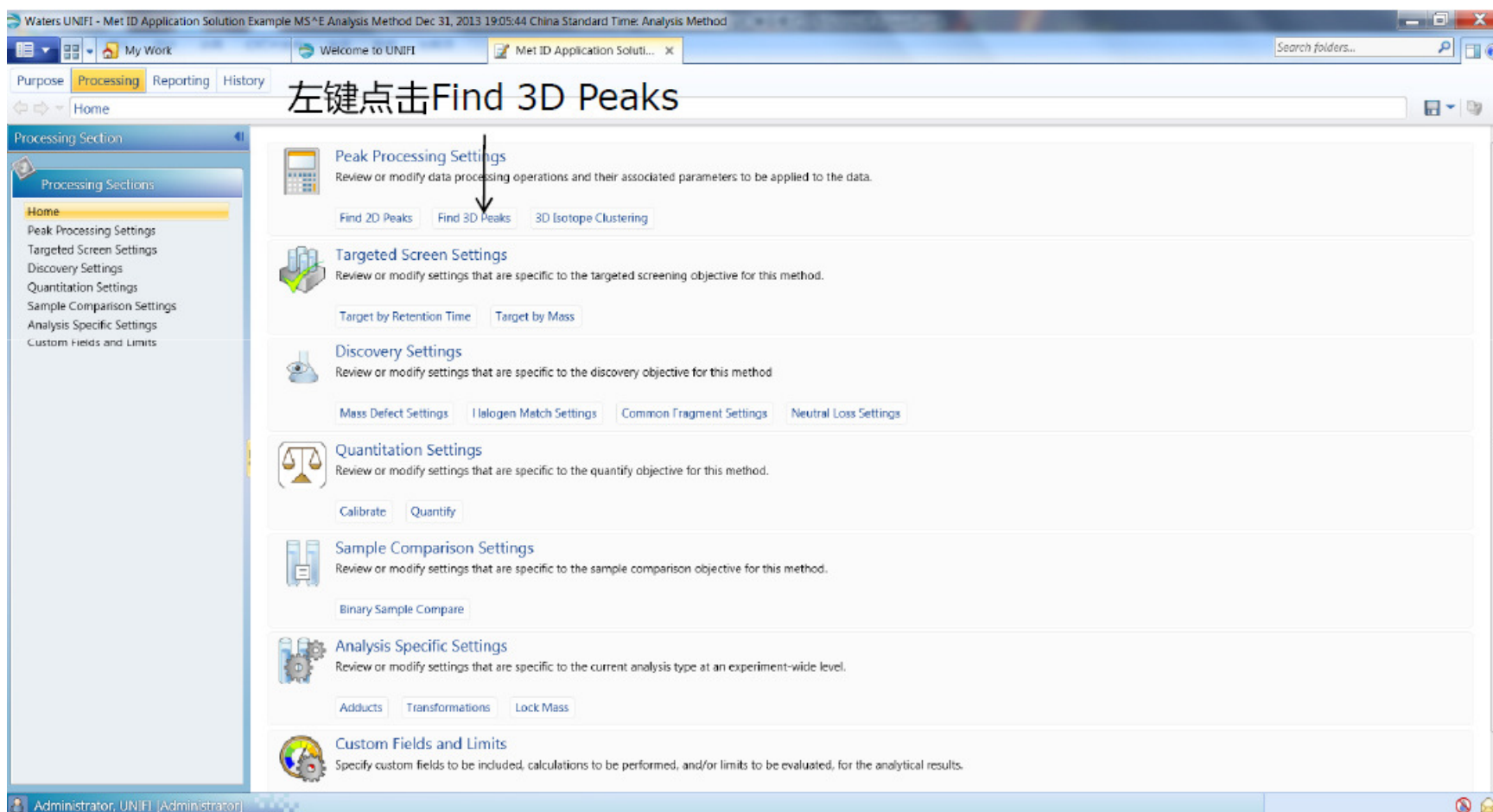
Create Import Paste Results Delete Edit Fragments...

| Component name | Label | Expected RT (min) | Expected neutral mass (Da) | Expected fragment (m/z) | Excluded | Formula | Internal standard? | Use internal standard | Use calibration curve | Calibration response |
|----------------|-------|-------------------|----------------------------|-------------------------|--------------------------|--------------|--------------------------|-----------------------|-----------------------|----------------------|
| 1 Nefazodone | | | 469.2245 | | <input type="checkbox"/> | C25H32ClN5O2 | <input type="checkbox"/> | | | |

Tips for adding expected components

Administrator, UNIFI [Administrator]

设置峰提取参数



设置峰提取参数

Waters UNIFI - Met ID Application Solution Example MSⁿE Analysis Method Dec 31, 2013 19:05:44 China Standard Time: Analysis Method

My Work Welcome to UNIFI Met ID Application Soluti...

Purpose Processing Reporting History

Home Peak Processing Settings

Category Navigation

- Find 3D Peaks
- Default settings
- Tasks
- 3D Peak Detection

点击返回

3D Peak Detection

Retention time range

Manually-specified retention time range

Start time: (Automatic) minutes

End time: (Automatic) minutes

Lock mass correction

Apply lock mass correction

MS resolution

Manually specified MS resolution

MS resolution: (Automatic)

Chromatographic peak width

Manually specified peak width

Peak width: (Automatic) minutes

High energy

Manually specified m/z range

Start m/z: (Automatic)

End m/z: (Automatic)

Intensity threshold: 5.0 counts

Low energy

Manually specified m/z range

Start m/z: (Automatic)

End m/z: (Automatic)

Intensity threshold: 20.0 counts

Noise

Background filter: High

Maximum number of peaks to keep per channel: 100000

Tips for setting 3D peak detection

Off

Low

Medium S/N > 3

High S/N > 10

High energy Intensity threshold / Low energy Intensity threshold > 1/10

设置质量匹配参数

The screenshot displays the Waters UNIFI software interface. The window title is "Waters UNIFI - Met ID Application Solution Example MS^E Analysis Method Dec 31, 2013 19:05:44 China Standard Time: Analysis Method". The interface includes a navigation pane on the left with "Processing Section" selected, and a main content area with several settings panels. The "Targeted Screen Settings" panel is active, showing "Target by Retention Time" and "Target by Mass" buttons. A callout with a left-pointing arrow and the text "左键点击 Target by Mass" is positioned over the "Target by Mass" button. Other panels include "Peak Processing Settings", "Discovery Settings", "Quantitation Settings", "Sample Comparison Settings", "Analysis Specific Settings", and "Custom Fields and Limits". The system tray at the bottom shows "Administrator, UNIFI [Administrator]" and system icons.

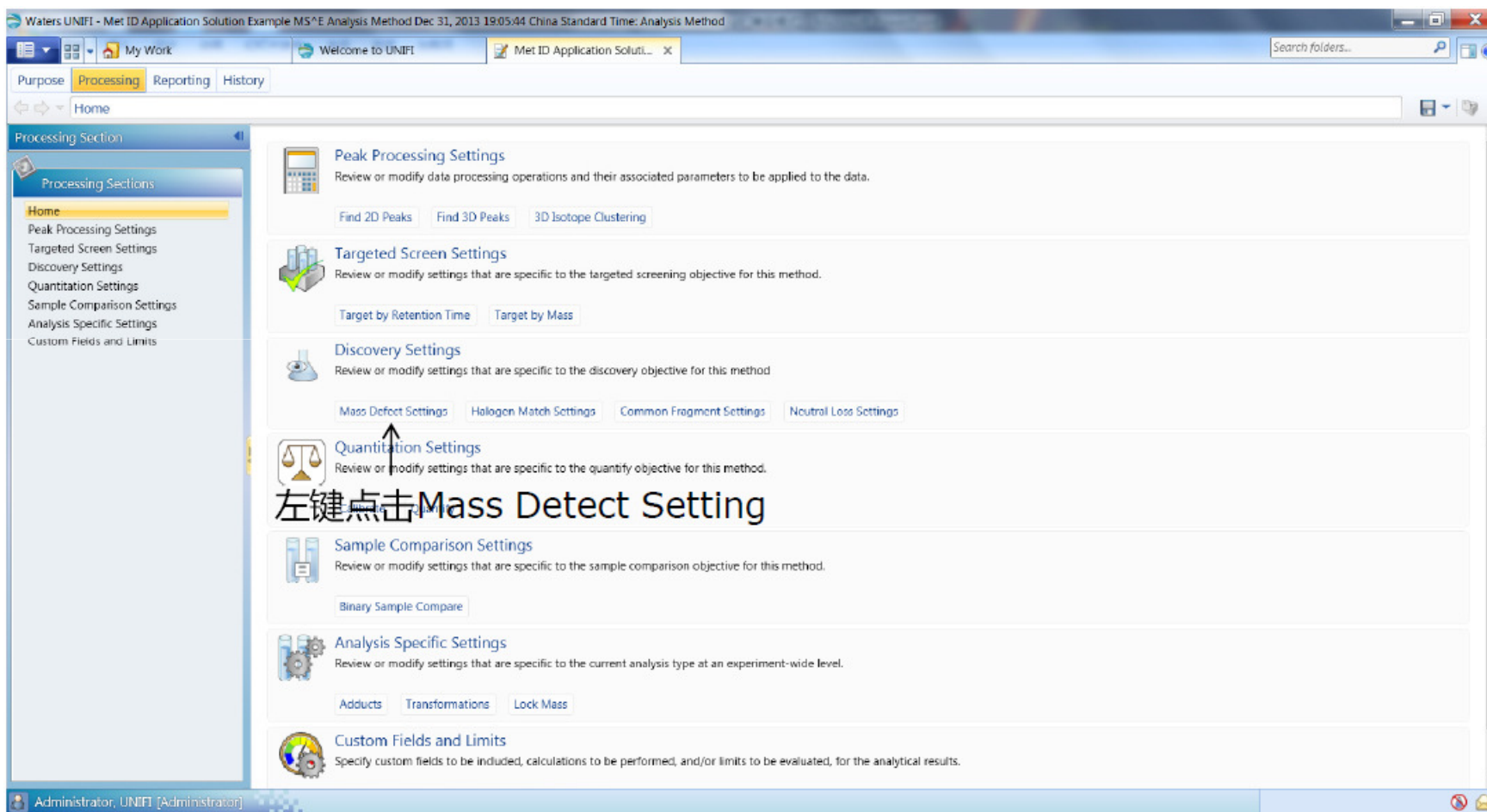
设置质量匹配参数

The screenshot displays the Waters UNIFI software interface. The window title is "Waters UNIFI - Met ID Application Solution Example MSⁿE Analysis Method Dec 31, 2013 19:05:44 China Standard Time: Analysis Method". The breadcrumb navigation shows "Home > Targeted Screen Settings". The left sidebar has a "Category Navigation" pane with "Targeted Screen Settings" selected. Under "Components", there is a button labeled "点击返回" (Click to return) and "Component defaults". The main content area is titled "Default Target by Mass" and contains the following settings:

- Target identification**
 - Mass units: PPM
 - Target match tolerance: 20.0
- Fragment identification**
 - Generate predicted fragments from structure
 - Fragment match tolerance: 2.0 mDa
 - Maximum allowed score: 8
- Detected components**
 - Extract mass chromatograms
 - Tolerance:
 - Automatic
 - Manual: 20.0 mDa
 - Extract a mass chromatogram containing all identified ions
- Undetected components**
 - Extract mass chromatograms
 - Extract separate mass chromatograms for each adduct
 - Extract summed mass chromatograms for all adducts
- Alternative assignments**
 - If more than one compound is assigned to a detected component display:
 - Only the best matching compound
 - All matching compounds
- Maximum candidates per sample to use during screening and discovery: 50000
- Maximum candidates per sample to keep after screening and discovery: 25000

At the bottom of the settings area, there is a link: [Define targeted screen component processing](#)

设置质量亏损 (MDF) 参数



设置质量亏损参数

The screenshot displays the Waters UNIFI software interface for configuring mass defect parameters. The main window is titled "Waters UNIFI - Met ID Application Solution Example MS^E Analysis Method Dec 31, 2013 19:05:44 China Standard Time. Analysis Method". The navigation pane on the left shows "Home" > "Discovery Settings" > "Mass Defect Search Settings" selected. A button labeled "点击返回" (Click to return) is visible in the left pane.

The "Mass Defect" configuration panel includes the following settings:

- Enable mass defect
- Selected adduct: +H
- Filter type: Cluster (selected), with a checkbox for Use ellipsoid
- Mass padding: 1 Da
- Defect padding: 50.0 mDa

Below the settings, there is a section for "Specify characteristic ions for component discovery".

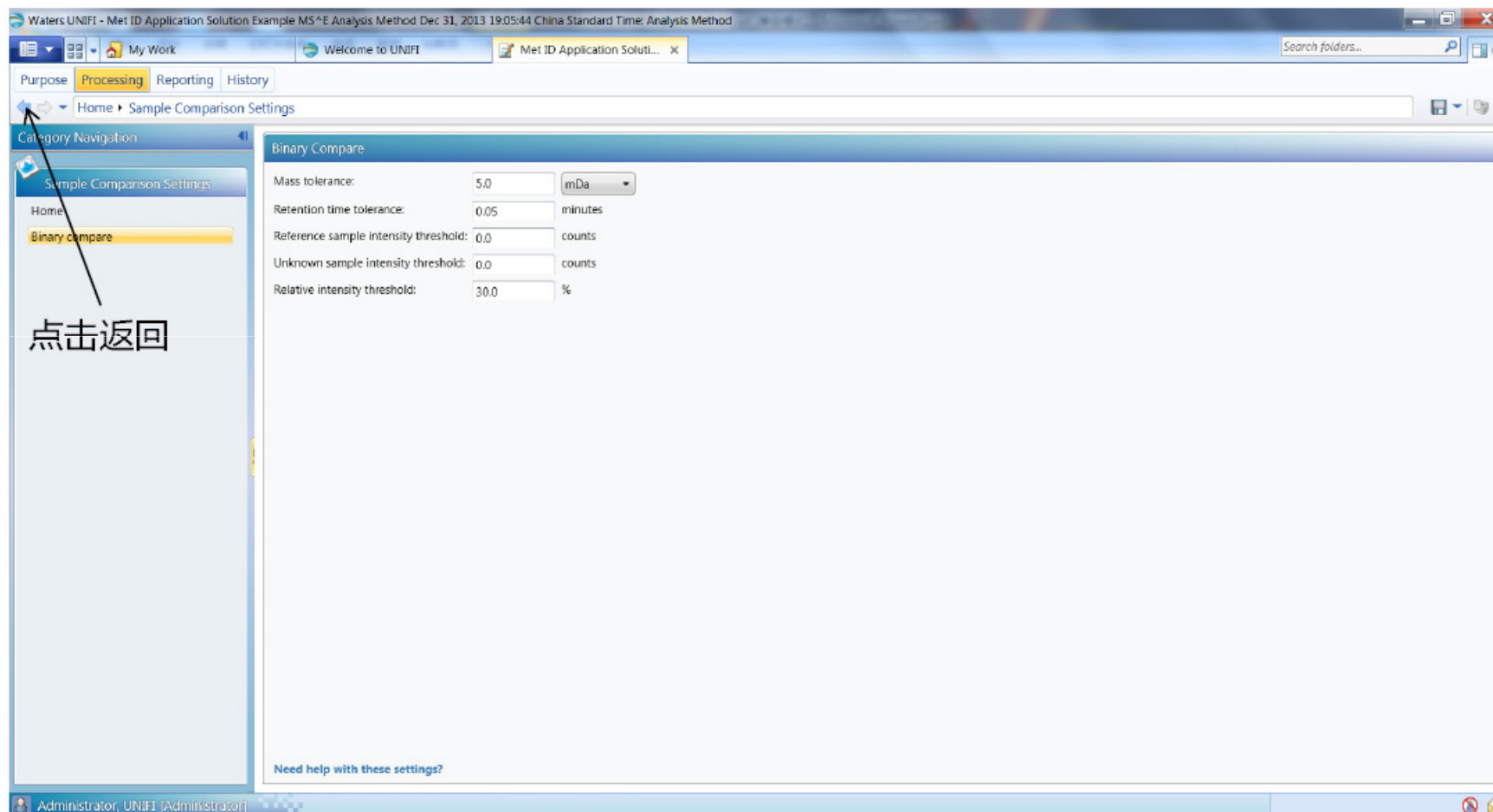
Two plots are shown on the right:

- The top plot, titled "Mass Defect Filter Applied", shows a mass defect plot with a blue shaded region representing the filter. The y-axis is labeled "Mass defect" and ranges from 0.000 to 0.300. The x-axis is labeled "m/z" and ranges from 100 to 700.
- The bottom plot shows a mass defect plot with a green shaded region representing the filter. The y-axis is labeled "Mass defect" and ranges from 0 to 150. The x-axis is labeled "Mass (Da)" and ranges from 20 to 500. A chemical structure is shown in the top left corner of this plot.

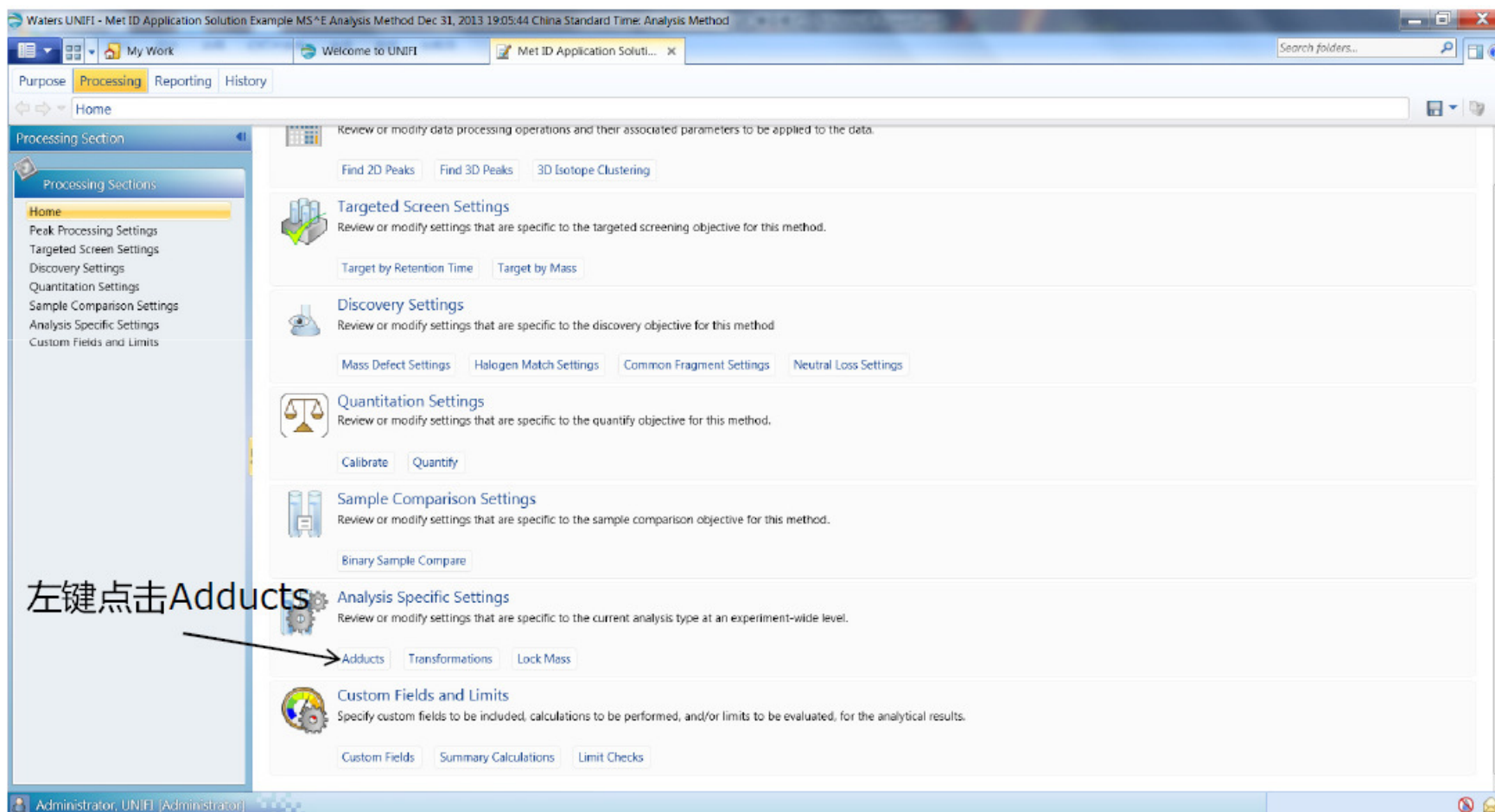
设置二元比较方法



二元比较



设置加和离子



加和离子

Waters UNIFI - Met ID Application Solution Example MSⁿE Analysis Method Dec 31, 2013 19:05:44 China Standard Time: Analysis Method

My Work Welcome to UNIFI Met ID Application Soluti...

Purpose Processing Reporting History

Home Analysis Specific Settings

Category Navigation

Analysis Specific Settings

Home

Adducts

Transformations

Lock mass

点击返回

Adducts

Select adducts to identify targeted components in positive and negative polarity mass data.

Available positive adducts

| Name | Delta Mass (Da) | Formula | Charge |
|------|-----------------|---------|--------|
| +H | 1.0073 | +H | 1 |
| +K | 38.9632 | +K | 1 |
| +Li | 7.0155 | +Li | 1 |
| -e | -0.0005 | -e | 1 |

Selected positive adducts

| Name | Delta Mass (Da) | Formula | Charge |
|------|-----------------|---------|--------|
| +H+ | 1.0073 | +H | 1 |
| +Na | 22.9892 | +Na | 1 |
| +NH4 | 18.0338 | +NH4 | 1 |

Available negative adducts

| Name | Delta Mass (Da) | Formula | Charge |
|---------|-----------------|---------|--------|
| +CH3COO | 59.0139 | +CH3COO | -1 |
| +Cl | 34.9694 | +Cl | -1 |
| +e | 0.0005 | +e | -1 |
| +HCOO | 44.9982 | +HCOO | -1 |
| -H | -1.0073 | -H | -1 |

Selected negative adducts

| Name | Delta Mass (Da) | Formula | Charge |
|------|-----------------|---------|--------|
| -H+ | -1.0073 | -H | -1 |

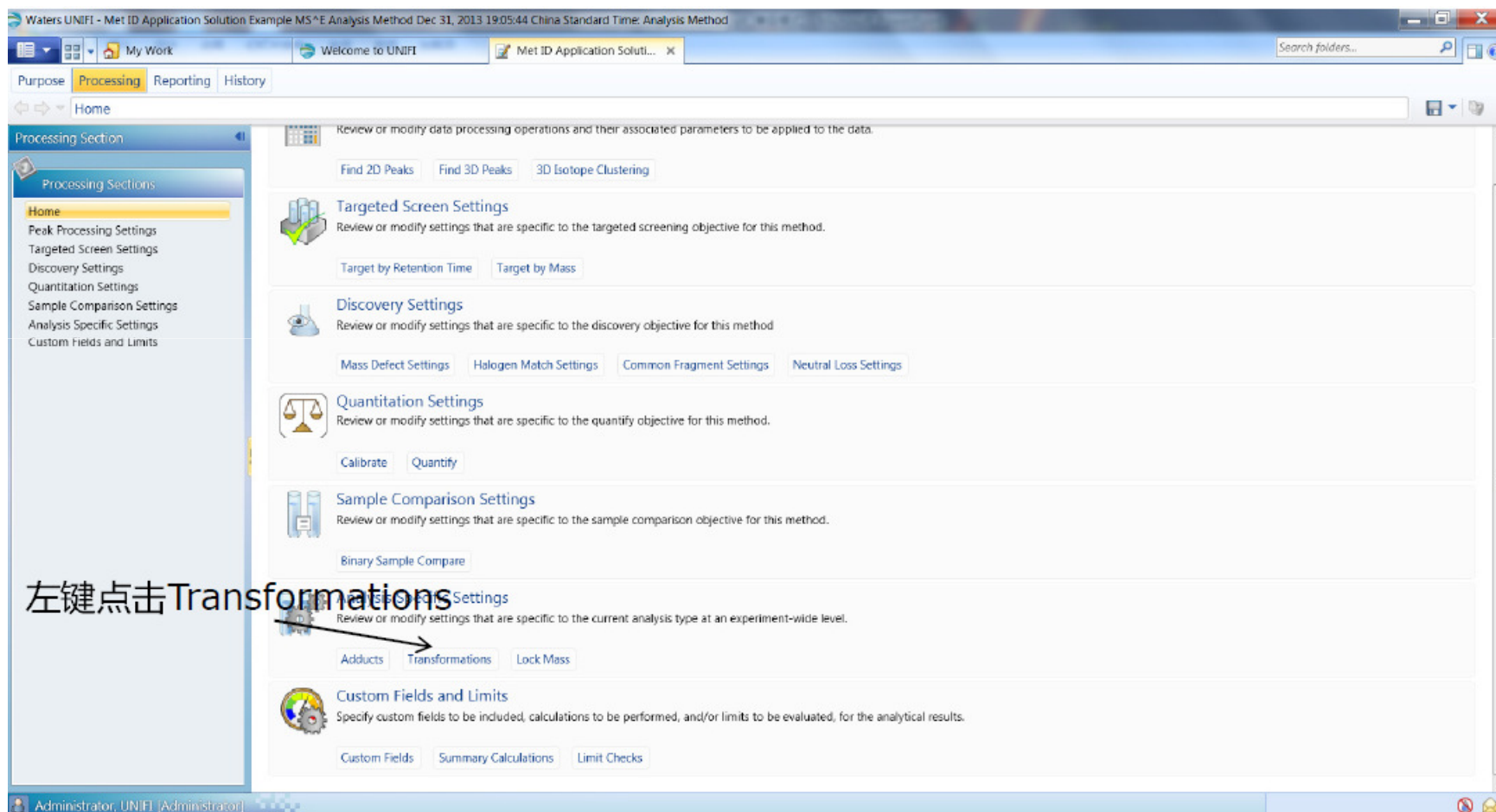
1 Maximum allowed absolute charge for adduct combinations

Allow cross adduct combinations

Specify adducts for component identification

Administrator, UNIFI [Administrator]

编辑代谢基团



编辑代谢基团

Waters UNIFI - Met ID Application Solution Example MS^E Analysis Method Dec 31, 2013 19:05:44 China Standard Time: Analysis Method

My Work Welcome to UNIFI Met ID Application Soluti...

Purpose Processing Reporting History

Home Analysis Specific Settings

Category Navigation

Analysis Specific Settings

Home

Adducts

Transformations

Lock mass

点击返回

Transformations

Select the transformations that you want to account for when identifying the target components within your samples.

| Available transformations | Name | Delta Mass (Da) | Formula | Classifier |
|---------------------------|------------------------------|-----------------|------------|------------|
| 1 | 2 x Debromination | -157.8367 | -Br2 | Phase I |
| 2 | 2 x Dechlorination | -69.9377 | -Cl2 | Phase I |
| 3 | 2 x Defluorination | -37.9968 | -F2 | Phase I |
| 4 | 2 x Glucuronide conjugation | 52.0642 | +C12H16O12 | Phase II |
| 5 | 2 x O-sulfate conjugation | 191.9035 | +S2O8 | Phase I |
| 6 | 2 x Oxidation | 31.9898 | +O2 | Phase I |
| 7 | 2 x Reductive debromination | -155.021 | -Br2 + H2 | Phase I |
| 8 | 2 x Reductive dechlorination | -67.922 | -Cl2 + H2 | Phase I |
| 9 | 2 x Reductive defluorination | -35.9811 | -F2 + H2 | Phase I |
| 10 | 2 x Sulfate conjugation | 159.9136 | +S2O6 | Phase II |
| 11 | 2-ethoxyl to acid | -0.0364 | -CH4 + O | Phase I |
| 12 | 3 x Oxidation | 47.9847 | +O3 | Phase I |

| Selected transformations | Name | Delta Mass (Da) | Formula | Classifier |
|--------------------------|---------------|-----------------|---------|------------|
| 1 | Hydroxylation | 15.9949 | +O | Phase I |

Maximum number of transformations:

Phase I: 1

Phase II: 0

Filter transformation list based on functional groups that are present

Run the dealkylation tool

Localize transformations

Maximum number of fragment peaks to consider: 10

Specify a trapping agent

Cyano

脱烷基化

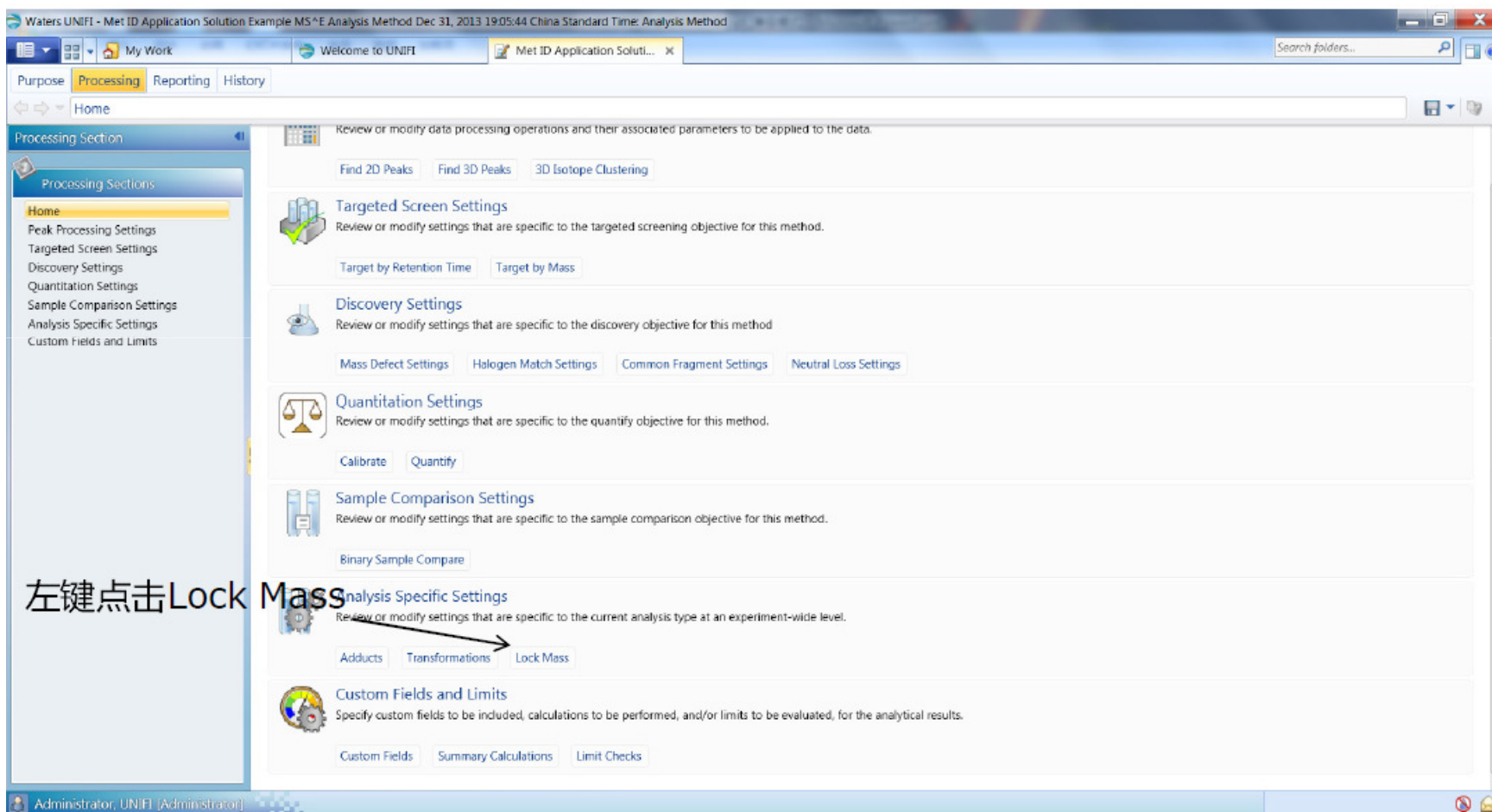
预测代谢位点

添加代谢基团

The screenshot shows the Waters UNIFI Scientific Library interface. The 'Scientific Library' tab is selected in the top navigation bar. The left sidebar shows the 'Modifications' link highlighted. The main content area displays a table of modifications with the following data:

| | Mass (g/mol) | Formula | Description | Classifiers |
|----|--------------|------------|-----------------------------------|-------------------------------|
| 1 | 194.08440 | +C13H10N2 | 2AAc | Fluorescent Labelling Reagent |
| 2 | 120.06875 | +C7H8N2 | 2AB | Fluorescent Labelling Reagent |
| 3 | -0.03640 | -CH4+O | 2-ethyl to acid | Phase I |
| 4 | 119.08473 | +C7H9N3-O | 4AB | Fluorescent Labelling Reagent |
| 5 | 128.07383 | +C9H8N2-O | 6AQ | Fluorescent Labelling Reagent |
| 6 | 121.05276 | +C7H7NO | AA | Fluorescent Labelling Reagent |
| 7 | 42.01060 | +C2H2O | Acetylation | Phase II |
| 8 | -2.01570 | -H2 | Alcohol to ketone | Phase I |
| 9 | -18.01060 | -H2O | Alcohols dehydration | Phase I |
| 10 | 34.00550 | +H2O2 | Alkenes to dihydrodiol | Phase I |
| 11 | 159.06841 | +C10H9NO | AMC | Fluorescent Labelling Reagent |
| 12 | 47.98470 | +O3 | Aromatic thiols to sulfonic acids | Phase I |
| 13 | -6.04700 | -H6 | Aromatization of saturated ring | Phase I |
| 14 | 70.04190 | +C4H6O | Butyryl conjugation | Phase II |
| 15 | 144.10250 | +C7H14O2N | Carnitine conjugation | Phase II |
| 16 | 24.99520 | +CN-H | Cyano | Metabolite Trapping Agent |
| 17 | 103.00920 | +C3H5NOS | Cysteine conjugation | Phase II |
| 18 | 93.06908 | +C5H7N3-O | DAP | Fluorescent Labelling Reagent |
| 19 | 295.11816 | +C14H13N7O | DAPMAB | Fluorescent Labelling Reagent |
| 20 | -90.04700 | -C7H6 | Debenzylation | Phase I |
| 21 | -78.91830 | -Br | Debromination | Phase I |
| 22 | -157.83670 | -Br2 | 2 x Debromination | Phase I |
| 23 | -27.99490 | -CO | Decarbonylation | Phase I |

设置lockmass



Waters UNIFI - Met ID Application Solution Example MS*E Analysis Method Dec 31, 2013 19:05:44 China Standard Time: Analysis Method

My Work Welcome to UNIFI Met ID Application Soluti... x Search folders...

Purpose Processing Reporting History

Home Analysis Specific Settings

Category Navigation

- Analysis Specific Settings
- Home
- Adducts
- Transformations
- Lock mass

Lock Mass Settings

Lock mass

Combine width: 3 scans

Mass window: 0.5 m/z

Reference mass 1: 556.276575 m/z (optional)

Reference charge 1: 1 (optional)

Reference mass 2: m/z (optional)

Reference charge 2: 1 (optional)

Optional fields only required if overriding acquired settings or when using MassLynx acquired data.

MS resolution

Manually specified MS resolution

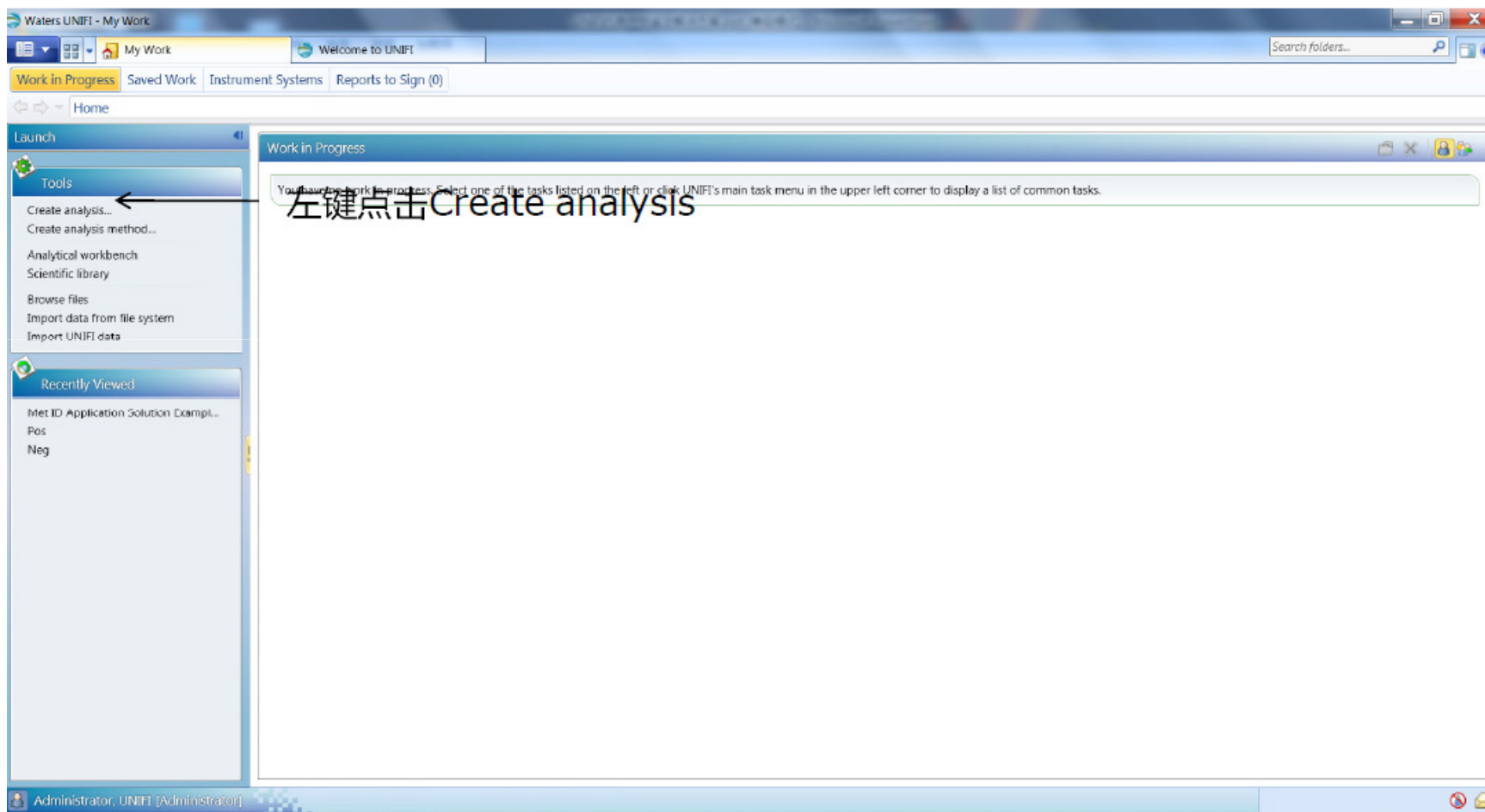
MS resolution: (Automatic)

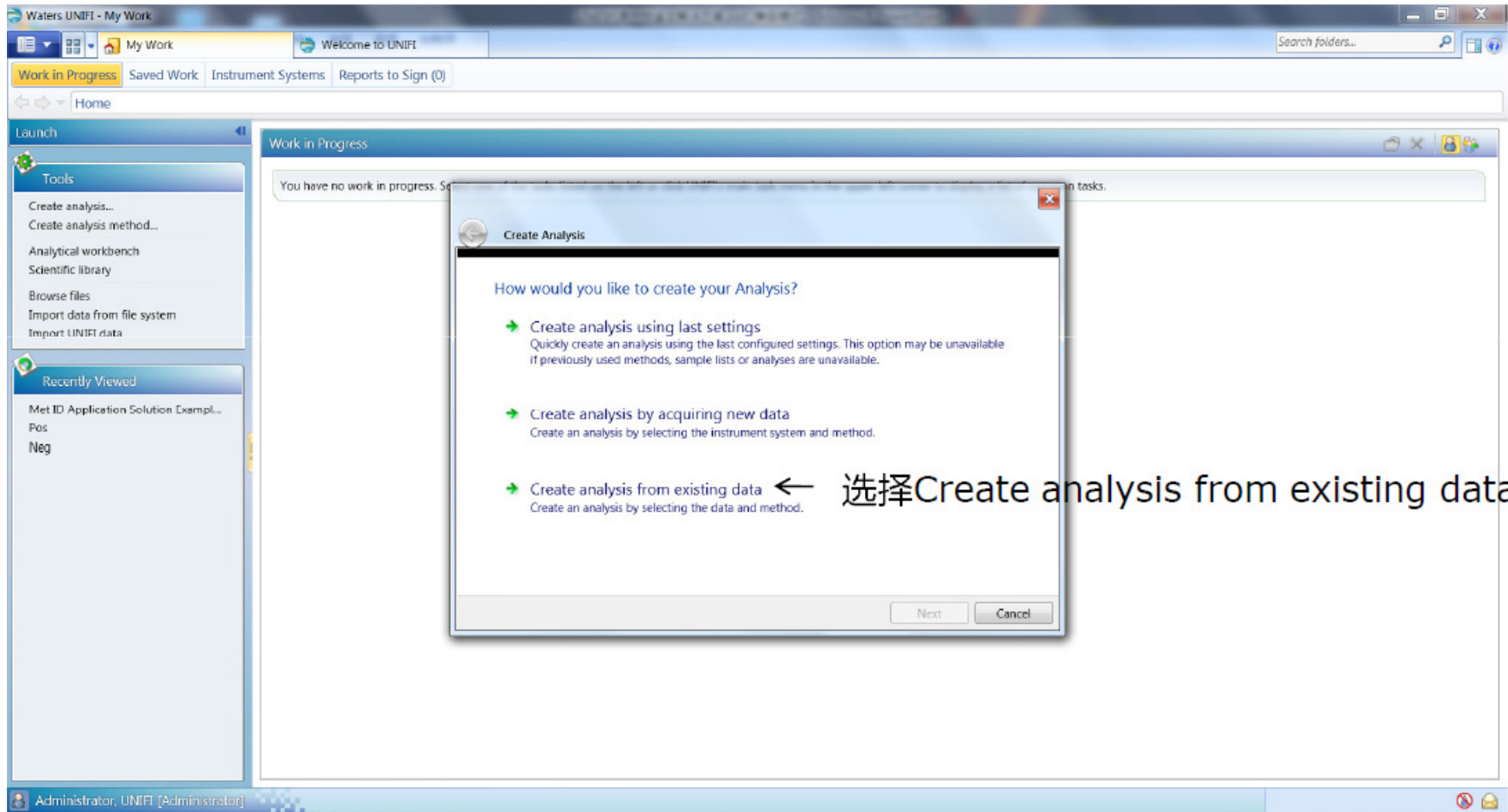
Need help defining settings?

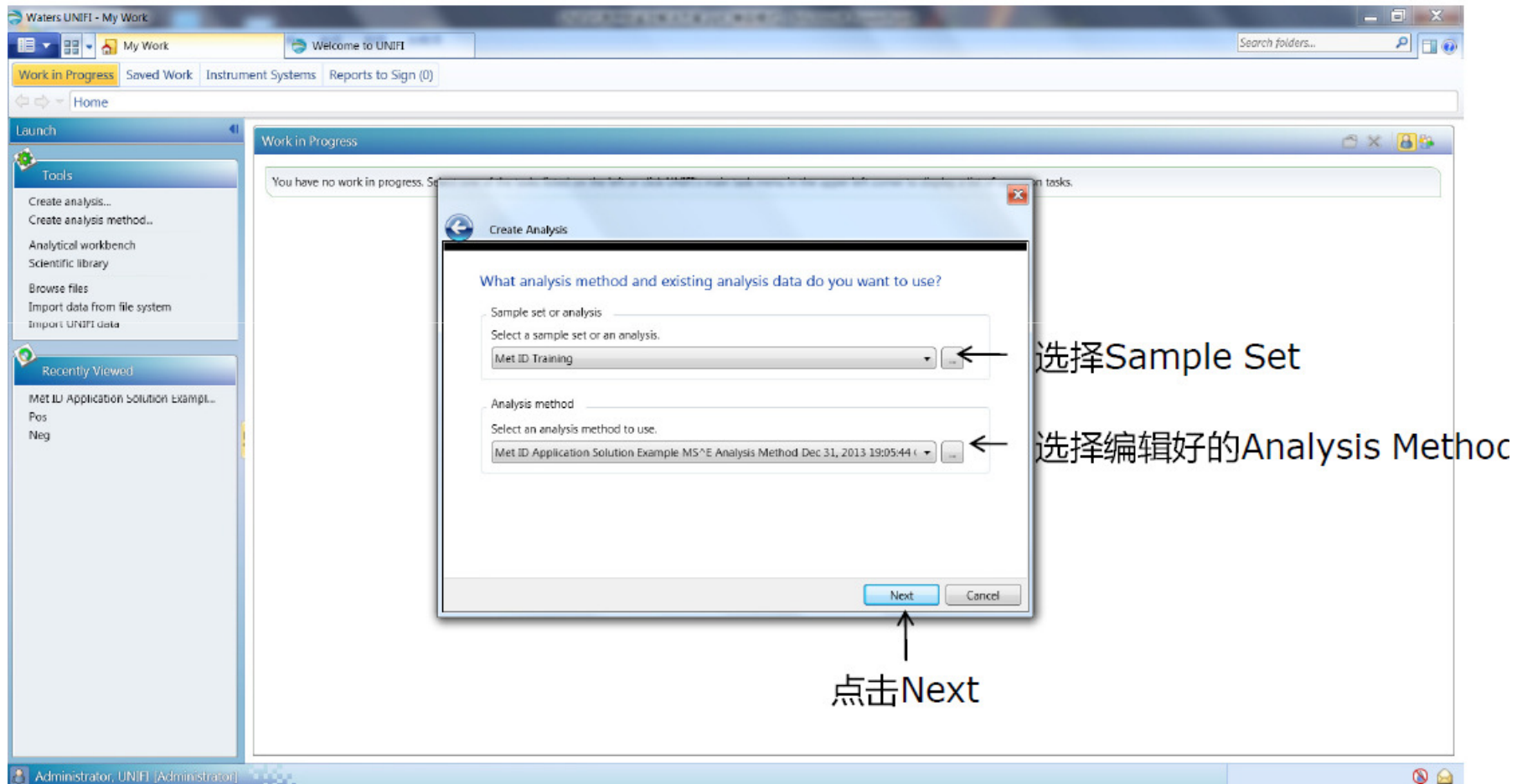
Administrator, UNIFI [Administrator]

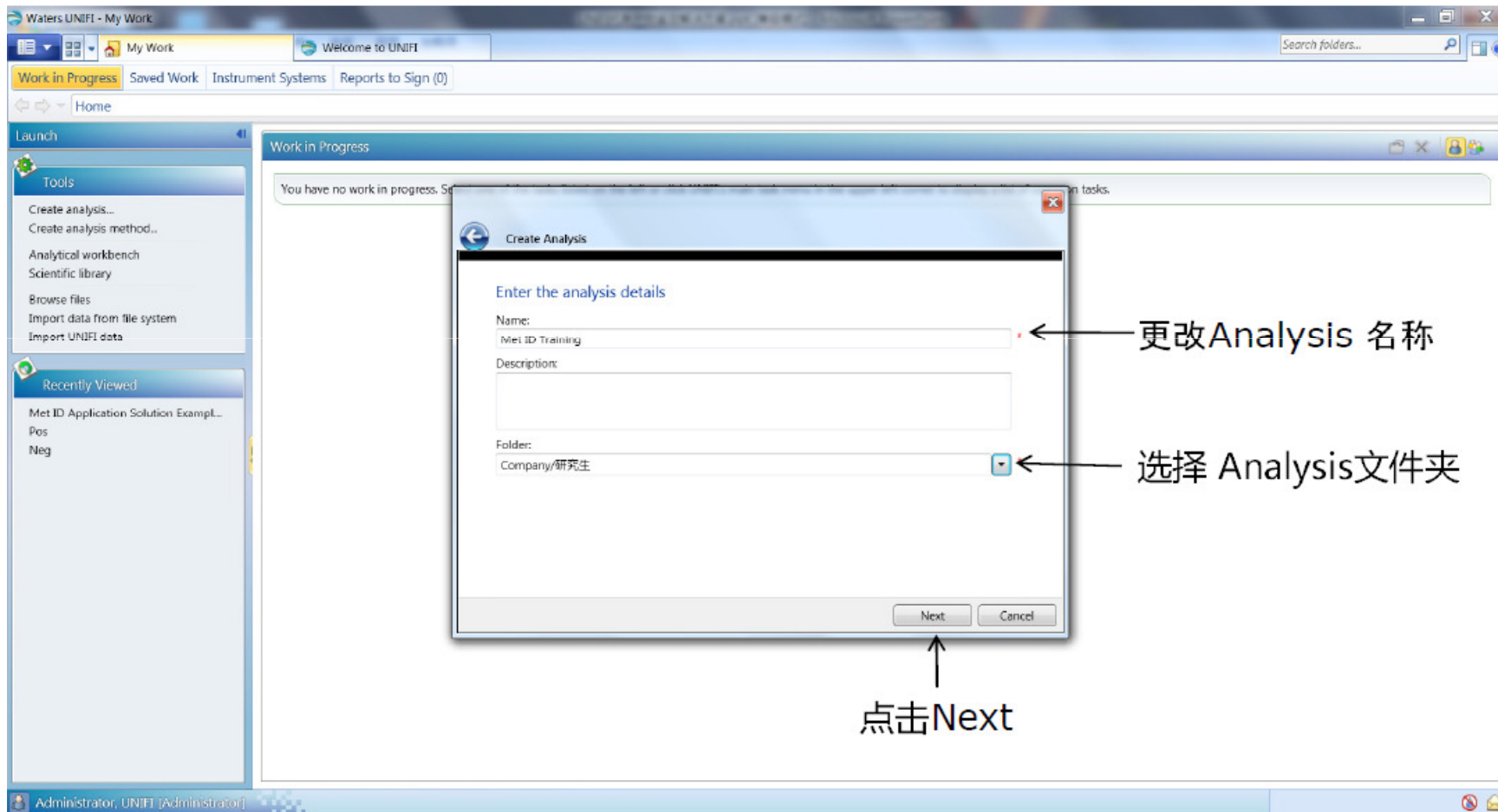
点击返回

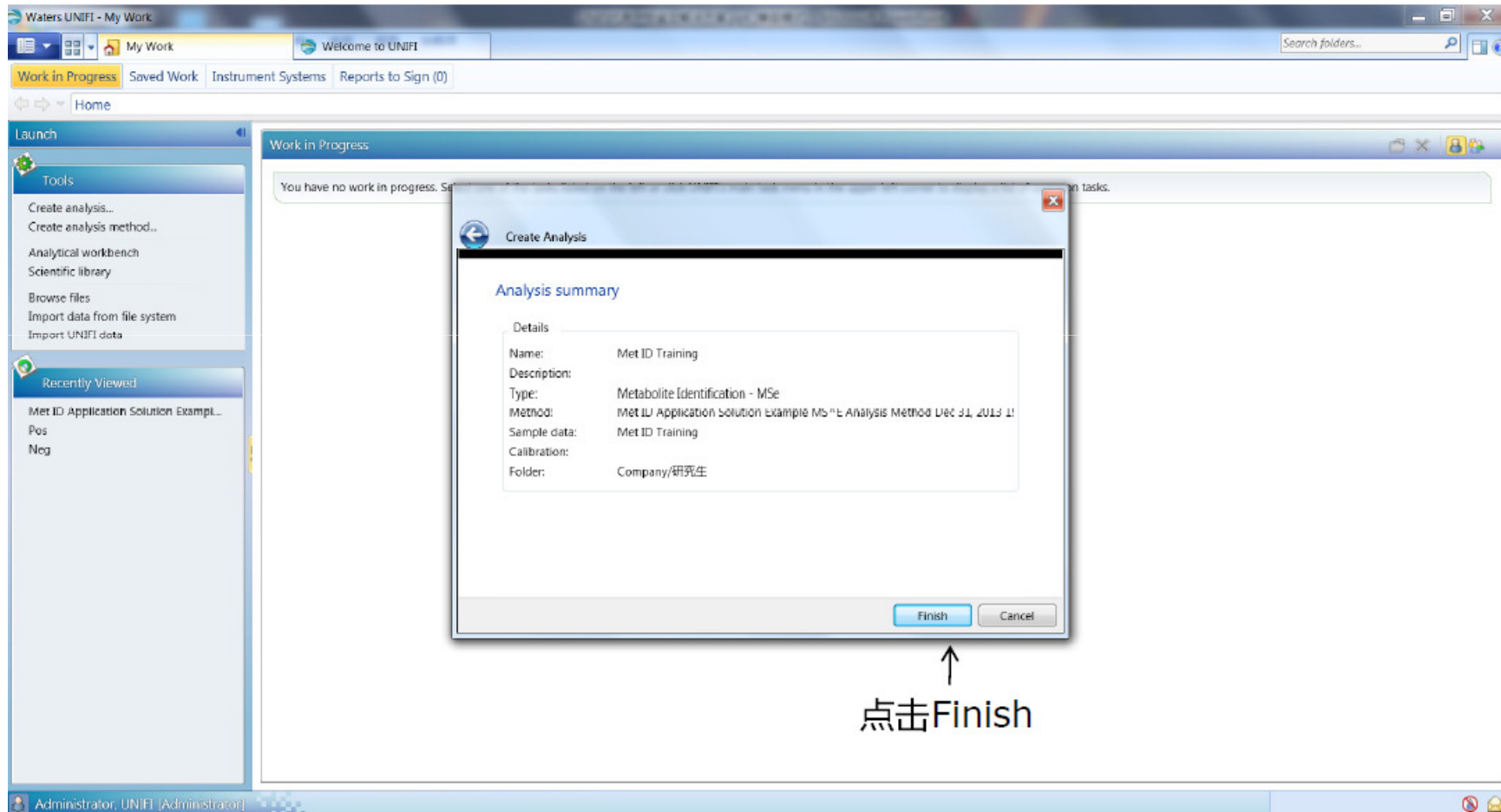
创建分析

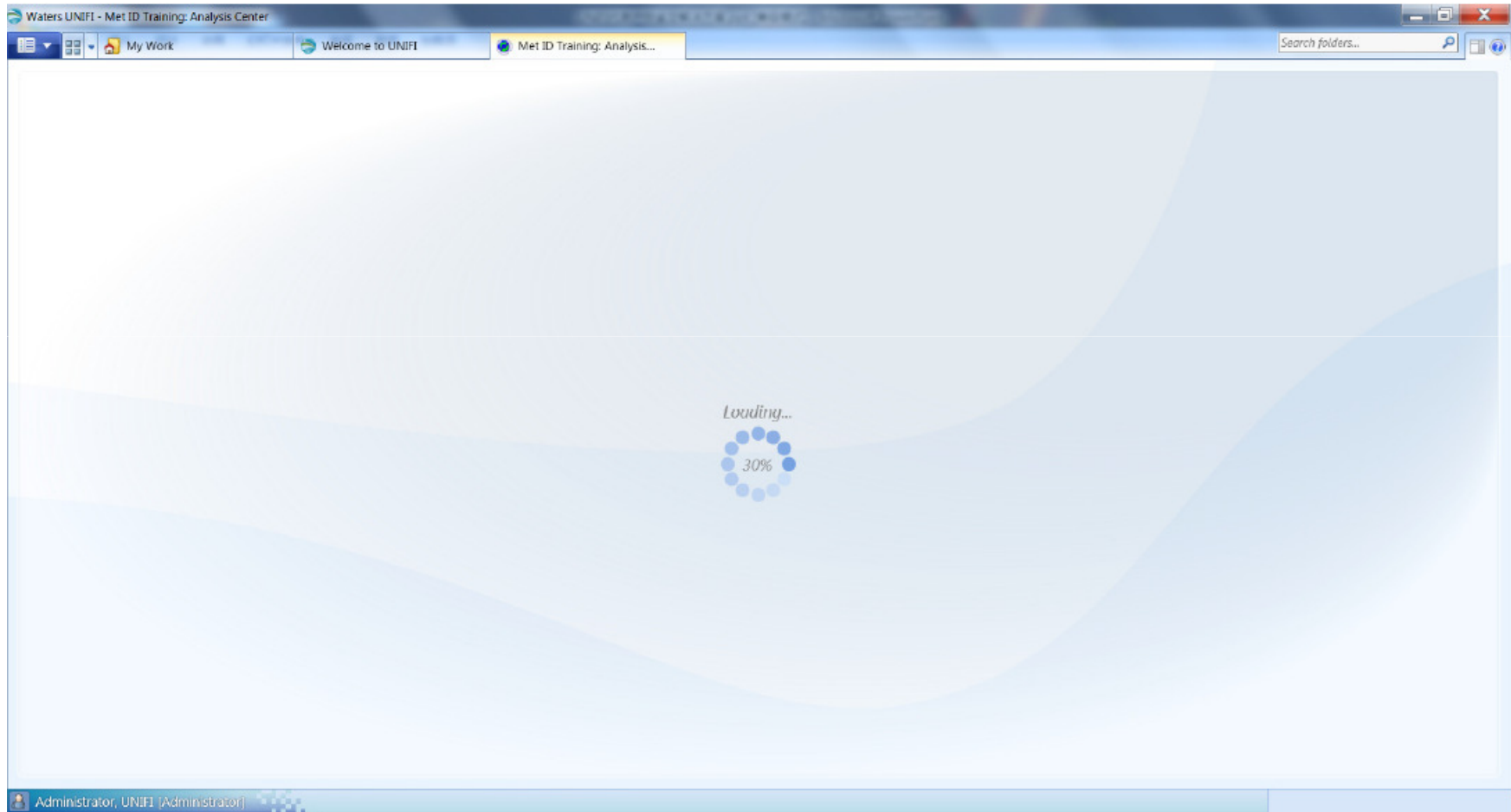




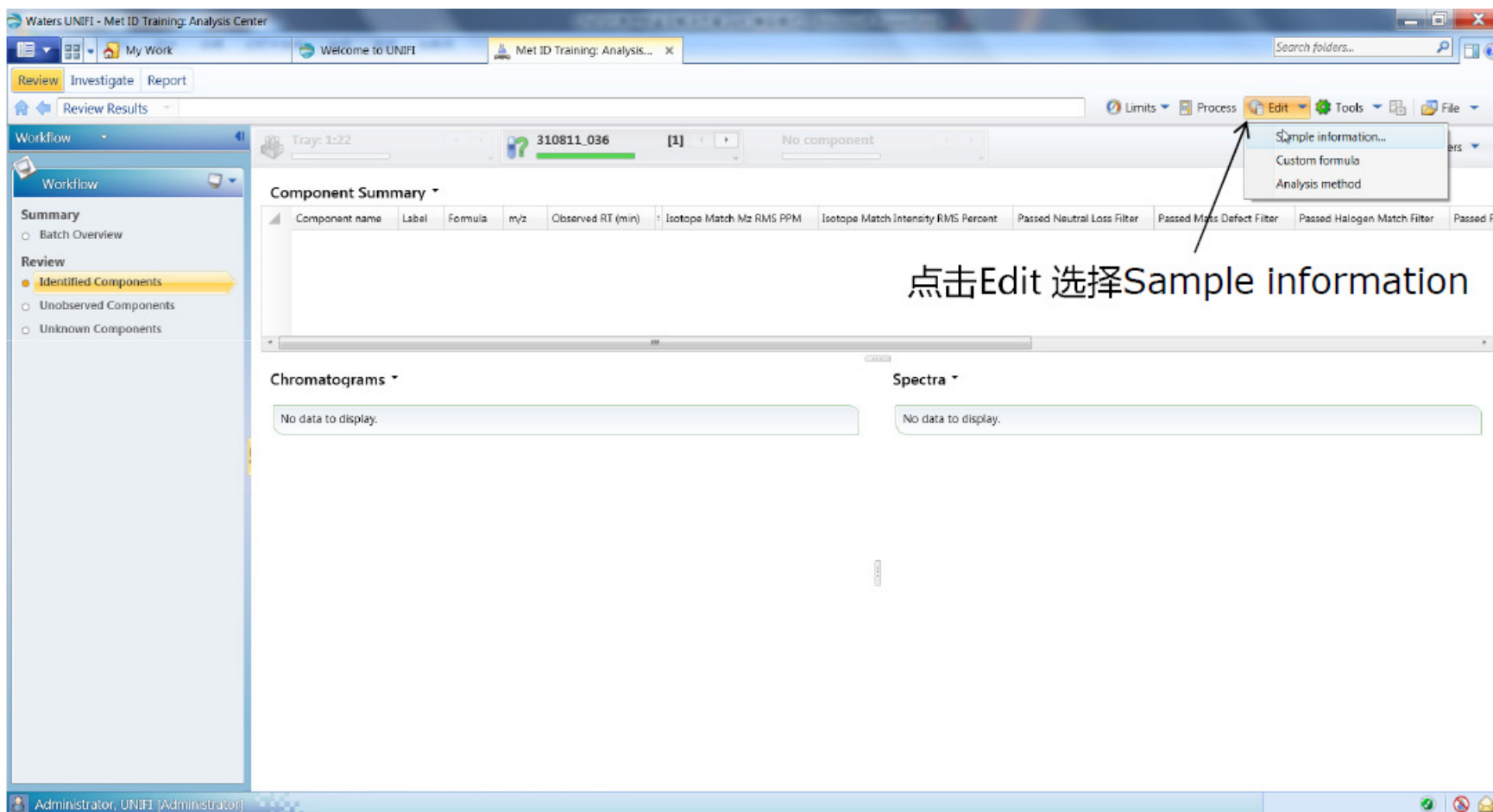








编辑样品信息

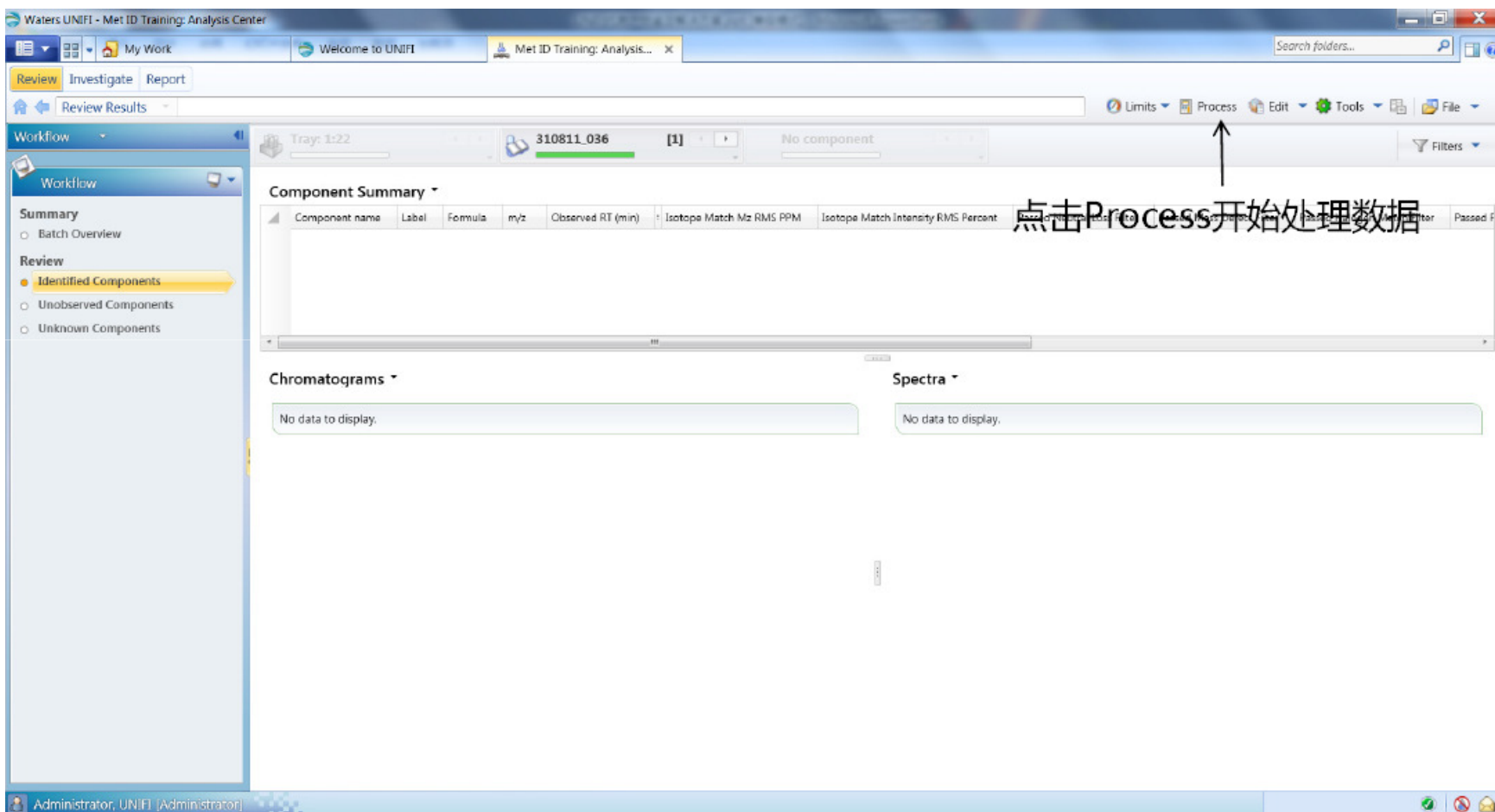


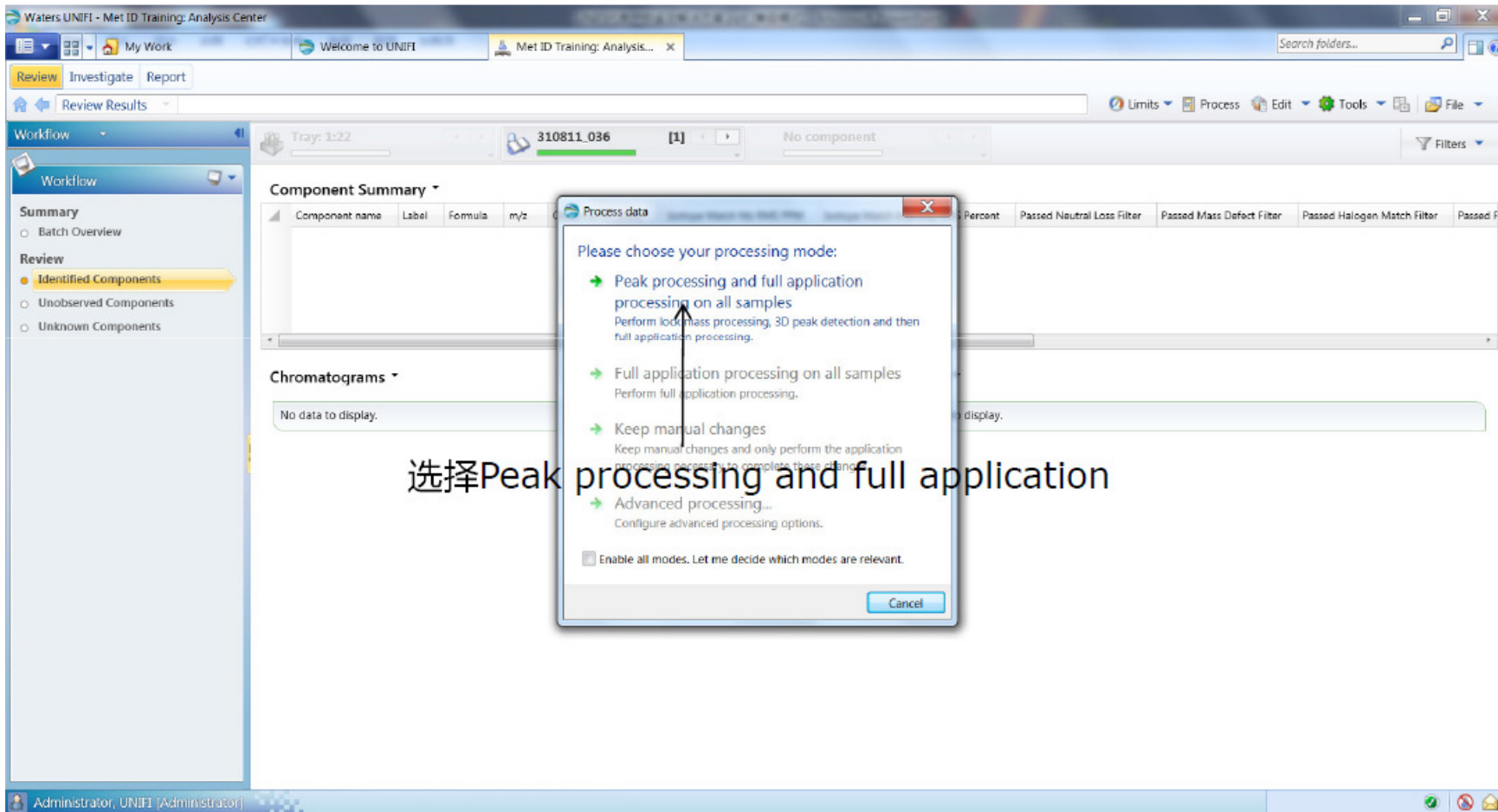
0时间点的样品Sample type改成Reference

| Sample Name | Sample type | Level | Sample position | Description | Replicates | Sample weight | Dilution factor |
|-------------|-------------|-------|-----------------|--|------------|---------------|-----------------|
| 310811_036 | Reference | 1:22 | | Nefazodone T0, 10 x diluted with water | 1 | | |
| 310811_037 | Unknown | 1:23 | | Nefazodone T5, 10 x diluted with water | 1 | | |
| 310811_038 | Unknown | 1:24 | | Nefazodone T15, 10 x diluted with water | 1 | | |
| 310811_039 | Unknown | 1:25 | | Nefazodone T30, 10 x diluted with water | 1 | | |
| 310811_040 | Unknown | 1:26 | | Nefazodone T45, 10 x diluted with water | 1 | | |
| 310811_041 | Unknown | 1:27 | | Nefazodone T45 - cofactor, 10 x diluted with water | 1 | | |
| 310811_042 | Unknown | 1:28 | | Nefazodone T45 - microsomes, 10 x diluted with water | 1 | | |
| 310811_043 | Unknown | 1:29 | | Nefazodone T60, 10 x diluted with water | 1 | | |
| 310811_044 | Unknown | 1:30 | | Nefazodone T120, 10 x diluted with water | 1 | | |

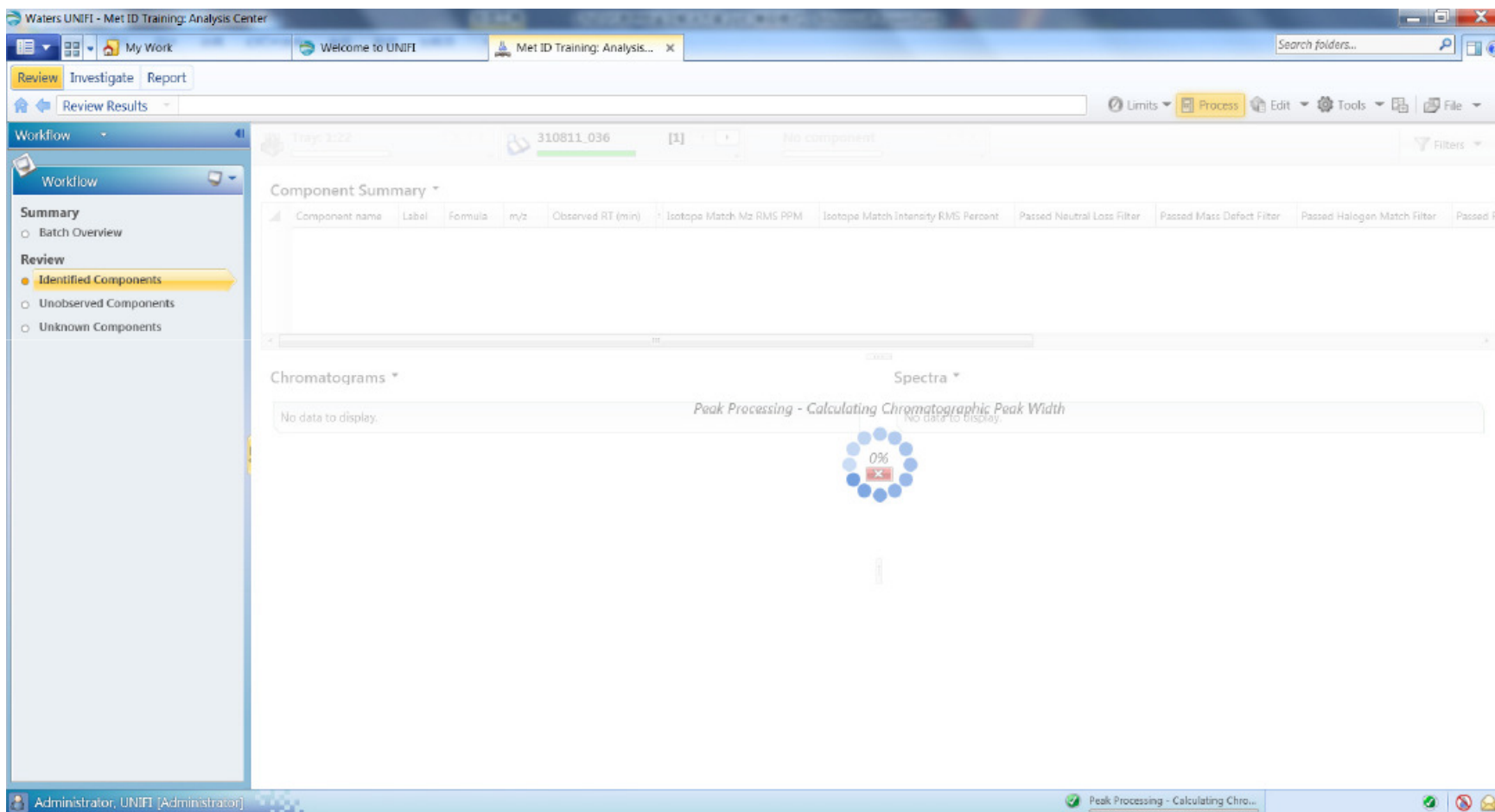
点击OK

开始处理数据





数据开始处理



导入workflow

The screenshot displays the Waters UNIFI software interface. The top navigation bar includes 'Review', 'Investigate', and 'Report' tabs. The main workspace shows a 'Component Summary' section with a context menu open over it. The menu options are: 'Save view', 'Save view as...', 'Manage views...', 'Customize workflow steps...', 'Import workflow...', and 'Export workflow...'. An arrow points to the 'Import workflow...' option, with the Chinese text '选择Import workflow' (Select Import workflow) next to it. Below the menu, there are two plots: 'Chromatograms' and 'Spectra'. The 'Chromatograms' plot shows a single sharp peak at approximately 3.2680 minutes. The 'Spectra' plot shows the mass spectrum of the peak, with the base peak at m/z 470.23166. The x-axis is 'Observed mass [m/z]' and the y-axis is 'Intensity [Counts]'. The bottom status bar shows the user is 'Administrator, UNIFI [Administrator]'.

The screenshot displays the Waters UNIFI - Met ID Training: Analysis Center interface. The main window shows a 'Component Summary' section with a note: 'Compare Results only available between Reference and Unknown samples'. An 'Open' file dialog is overlaid on the center, showing the file 'Metabolite Identification Workflow.xml' selected in the 'Workflows' folder. The dialog's file name field contains 'Metabolite Identification Workflow.xml' and the file type is set to 'XML file (xml) (*.xml)'. The background shows a mass spectrum plot with 'Intensity [Counts]' on the y-axis and 'Observed mass [m/z]' on the x-axis. The plot features several peaks, with the most prominent one at m/z 470.23166. Other labeled peaks include 469.20531, 472.22918, 473.23145, 492.21384, and 596.36158. The x-axis ranges from 400 to 600 m/z, and the y-axis ranges from -5e5 to 5e5. The software interface also shows a 'Workflow' sidebar on the left with options like 'Batch Overview', 'Identified Components', 'Unobserved Components', and 'Unknown Components'. The top status bar indicates 'Tray: 1:22', '310811_036 [1]', and 'Nefazodone'.

选择 Metabolite Identification Workflow.xml

Waters UNIFI - Met ID Training: Analysis Center

My Work Welcome to UNIFI Met ID Training: Analysis...

Review Investigate Report

Review Results

Workflow Tray: 1:22 310811_036 [1] Nefazodone

Component Summary

| Component name | Label | Formula | m/z | Observed RT (min) | Isotope Match Mz RMS PPM | Isotope Match Intensity RMS Percent | Passed Neutral Loss Filter | Passed Mass Defect Filter | Passed H |
|---------------------------------------|-------|--------------|----------|-------------------|--------------------------|-------------------------------------|----------------------------|-------------------------------------|----------|
| 1 Nefazodone | | C25H32ClN5O2 | 470.2317 | 3.27 | 0.71 | 1.55 | <input type="checkbox"/> | <input checked="" type="checkbox"/> | |
| 2 Nefazodone+O | | C25H32ClN5O3 | 486.2247 | 3.07 | 4.72 | 14.47 | <input type="checkbox"/> | <input checked="" type="checkbox"/> | |
| 3 Nefazodone-C11H12N2O(dealenylation) | | C14H20ClN3O | 299.1608 | 4.40 | 9.06 | 20.64 | <input type="checkbox"/> | <input checked="" type="checkbox"/> | |

Chromatograms

Item name: 310811_036
Channel name: Nefazodone (+H+): (0.0200 Da) 470.2317

Import Workflow

The workflow file contains views that match existing views. Do you want to overwrite the existing view data with the view data contained in the file?

Yes No

选择Yes

Item name: 310811_036
Channel name: Low energy: Time 3.2680 +/- 0.0098...
Description: Nefazodone TO, 10 x diluted with water

Item name: 310811_036
Channel name: High energy: Time 3.2680 +/- 0.0098...
Description: Nefazodone TO, 10 x diluted with water

Administrator, UNIFI [Administrator]

处理结果浏览

Waters UNIFI - Met ID Training: Analysis Center

Review Investigate Report

Review Results

Workflow ← 选择Injections and Components

Component Summary

| Component name | Label | Formula | m/z | Observed RT (min) | Isotope Match Mz RMS PPM | Isotope Match Intensity RMS Percent | Passed Neutral Loss Filter | Passed Mass Defect Filter |
|---------------------------------------|-------|--------------|----------|-------------------|--------------------------|-------------------------------------|----------------------------|-------------------------------------|
| 1 Nefazodone | | C25H32ClN5O2 | 470.2315 | 3.27 | 0.88 | 0.95 | <input type="checkbox"/> | <input checked="" type="checkbox"/> |
| 2 Nefazodone+O | | C25H32ClN5O3 | 486.2263 | 3.07 | 1.00 | 1.01 | <input type="checkbox"/> | <input checked="" type="checkbox"/> |
| 3 Nefazodone-C6H3Cl(dealkylation) | | C19H29N5O2 | 360.2386 | 2.13 | 2.09 | 5.30 | <input type="checkbox"/> | <input checked="" type="checkbox"/> |
| 4 Nefazodone-C15H19N3O2(dealkylation) | | C10H13ClN2 | 197.0835 | 2.11 | 2.41 | 13.24 | <input type="checkbox"/> | <input checked="" type="checkbox"/> |
| 5 Nefazodone+O | | C23H32ClN5O5 | 486.2248 | 2.93 | 5.76 | 4.69 | <input type="checkbox"/> | <input checked="" type="checkbox"/> |
| 6 Nefazodone-C6H3Cl(dealkylation)+O | | C19H29N5O3 | 376.2325 | 1.77 | 5.52 | 13.30 | <input type="checkbox"/> | <input checked="" type="checkbox"/> |
| 7 Nefazodone-C2H2(dealkylation) | | C23H30ClN5O2 | 444.2140 | 3.27 | 5.34 | 15.62 | <input type="checkbox"/> | <input checked="" type="checkbox"/> |
| 8 Nefazodone-C10H11ClN2(dealkylation) | | C15H12ClN3O3 | 292.1037 | 2.97 | 7.34 | 21.10 | <input type="checkbox"/> | <input checked="" type="checkbox"/> |
| 9 Nefazodone-C11H12N2O(dealkylation) | | C14H20ClN3O | 299.1623 | 4.41 | 4.96 | 20.30 | <input type="checkbox"/> | <input checked="" type="checkbox"/> |

Chromatograms

Item name: 310811_038
Channel name: Nefazodone+O [+H+] : (0.0200 Da) 486.2263

Spectra

Item name: 310811_038
Channel name: Low energy : Time 3.0711 +/- 0...
Description: Nefazodone T15, 10 x diluted with...

Waters UNIFI - Met ID Training: Analysis Center

My Work Welcome to UNIFI Met ID Training: Analysis...

Review Investigate Report

Review Results

Injections and Components

Reference

| Name | Description | Type | Acquisition status |
|------------|--|------|--------------------|
| 310811_036 | Nefazodone T0, 10 x diluted with water | | Complete |
| 310811_037 | Nefazodone T5, 10 x diluted with water | | Complete |
| 310811_038 | Nefazodone T15, 10 x diluted with water | | Complete |
| 310811_039 | Nefazodone T30, 10 x diluted with water | | Complete |
| 310811_040 | Nefazodone T45, 10 x diluted with water | | Complete |
| 310811_041 | Nefazodone T45 - cofactor, 10 x diluted with water | | Complete |
| 310811_042 | Nefazodone T45 - microsomes, 10 x diluted with water | | Complete |
| 310811_043 | Nefazodone T60, 10 x diluted with water | | Complete |
| 310811_044 | Nefazodone T120, 10 x diluted with water | | Complete |

Tray: 1:24 310811_038 [1] Nefazodone+O

Component Summary

| Component name | Label | Formula | m/z | Observed RT (min) | Isotope Match Mz RMS PPM | Isotope Match Intensity RMS Percent | Passed |
|----------------|--------------------------|--------------|----------|-------------------|--------------------------|-------------------------------------|--------|
| 1 | Nefazodone | C25H32ClN5O2 | 470.2315 | 3.27 | 0.88 | 0.95 | |
| 2 | Nefazodone+O | C25H32ClN5O3 | 486.2263 | 3.07 | 1.00 | 1.01 | |
| 3 | Nefazodone-C6H3Cl(dea... | C19H29N5O2 | 360.2386 | 2.13 | 2.09 | 5.30 | |
| 4 | Nefazodone-C15H19N3... | C10H13ClN2 | 197.0835 | 2.11 | 2.41 | 13.24 | |
| 5 | Nefazodone+O | C25H32ClN5O3 | 486.2248 | 2.93 | 3.76 | 4.69 | |
| 6 | Nefazodone-C6H3Cl(dea... | C19H29N5O3 | 376.2325 | 1.77 | 5.52 | 13.30 | |
| 7 | Nefazodone-C2H2(dealk... | C23H30ClN5O2 | 444.2140 | 3.27 | 5.34 | 15.62 | |
| 8 | Nefazodone C10H11ClN... | C15H21N3O3 | 292.1637 | 2.97 | 7.34 | 21.10 | |
| 9 | Nefazodone-C11H12N2... | C14H20ClN3O | 299.1623 | 4.41 | 4.96 | 20.30 | |

Unknown

Components (310811_038, Count: 9)

| Status | Label | Name | Observed RT (min) |
|--------|-------|---------------------------------------|-------------------|
| ✓ | | Nefazodone | 3.27 |
| ✓ | | Nefazodone+O | 3.07 |
| ✓ | | Nefazodone+O | 2.93 |
| ✓ | | Nefazodone-C15H19N3O2(dealkylation) | 2.11 |
| ✓ | | Nefazodone-C10H11ClN2(dealkylation)+O | 2.97 |
| ✓ | | Nefazodone-C11H12N2O(dealkylation) | 4.41 |
| ✓ | | Nefazodone-C6H3Cl(dealkylation) | 2.13 |
| ✓ | | Nefazodone-C6H3Cl(dealkylation)+O | 1.77 |
| ✓ | | Nefazodone-C2H2(dealkylation) | 3.27 |

Chromatograms

Item name: 310811_038
Channel name: Nefazodone+O [+H+]; (0.0200 Da) 486.2263

Spectra

Item name: 310811_038 Channel name: Low energy : Tim...
Description: Nefazodone T15, 1...

Administrator, UNIFI [Administrator]

Waters UNIFI - Met ID Training: Analysis Center

My Work | Welcome to UNIFI | Met ID Training: Analysis... | Search folders...

Review Investigate Report

Review Results

Workflow | 310811_038 [1] | Nefazodone+O

选择Workflow

Component Summary

| Component name | Label | Formula | m/z | Observed RT (min) | Isotope Match Mz RMS PPM | Isotope Match Intensity RMS Percent | Passed Neutral Loss Filter | Passed Mass Defect Filter | Passed Halogen Match |
|----------------|-------|--------------|----------|-------------------|--------------------------|-------------------------------------|----------------------------|-------------------------------------|-------------------------------------|
| 1 Nefazodone+O | | C25H32ClN5O3 | 486.2265 | 3.07 | 0.90 | 4.63 | <input type="checkbox"/> | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| 2 Nefazodone+O | | C25H32ClN5O3 | 486.2267 | 3.07 | 0.48 | 2.86 | <input type="checkbox"/> | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| 3 Nefazodone+O | | C25H32ClN5O3 | 486.2265 | 3.07 | 0.38 | 1.07 | <input type="checkbox"/> | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| 4 Nefazodone+O | | C25H32ClN5O3 | 486.2263 | 3.07 | 0.82 | 2.88 | <input type="checkbox"/> | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| 5 Nefazodone+O | | C25H32ClN5O3 | 486.2263 | 3.07 | 1.00 | 1.01 | <input type="checkbox"/> | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| 6 Nefazodone+O | | C25H32ClN5O3 | 486.2251 | 3.07 | 3.10 | 4.10 | <input type="checkbox"/> | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| 7 Nefazodone+O | | C25H32ClN5O3 | 486.2247 | 3.07 | 4.72 | 14.47 | <input type="checkbox"/> | <input checked="" type="checkbox"/> | <input type="checkbox"/> |

Chromatograms

Item name: 310811_038
Channel name: Nefazodone+O [+H+]: (0.0200 Da) 486.2263

Spectra

Item name: 310811_038
Channel name: Low energy : Time 3.0711 +/- 0.0...
Description: Nefazodone T15, 10 x diluted with...

Administrator, UNIFI [Administrator]

Waters UNIFI - Met ID Training: Analysis Center

My Work | Welcome to UNIFI | Met ID Training: Analysis... | Search folders...

Review | Investigate | Report

Review Results

Workflow

Tray: 1:23

310811_037 [1] Nefazodone+O

选择一个Unknown的样品

Component Summary

| Component name | Label | Formula |
|----------------|-------|---------|
| 1 Nefazodone+O | | C25H32O |
| 2 Nefazodone+O | | C25H32O |
| 3 Nefazodone+O | | C25H32O |
| 4 Nefazodone+O | | C25H32O |
| 5 Nefazodone+O | | C25H32O |
| 6 Nefazodone+O | | C25H32O |
| 7 Nefazodone+O | | C25H32O |
| 8 Nefazodone+O | | C25H32O |
| 9 Nefazodone+O | | C25H32O |

Injections 9/9

| Item name | Description |
|--------------|--|
| 1 310811_036 | Nefazodone T0, 10 x diluted with water |
| 2 310811_037 | Nefazodone T5, 10 x diluted with water |
| 3 310811_038 | Nefazodone T15, 10 x diluted with water |
| 4 310811_039 | Nefazodone T30, 10 x diluted with water |
| 5 310811_040 | Nefazodone T45, 10 x diluted with water |
| 6 310811_041 | Nefazodone T45 - cofactor, 10 x diluted with water |
| 7 310811_042 | Nefazodone T45 - microsomes, 10 x diluted with water |
| 8 310811_043 | Nefazodone T60, 10 x diluted with water |
| 9 310811_044 | Nefazodone T120, 10 x diluted with water |

| Match Intensity | RMS Percent | Passed Neutral Loss Filter | Passed Mass Defect Filter | Passed Halogen Mat |
|-----------------|-------------|----------------------------|-------------------------------------|-------------------------------------|
| 4.63 | | <input type="checkbox"/> | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| 2.86 | | <input type="checkbox"/> | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| 1.07 | | <input type="checkbox"/> | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| 2.88 | | <input type="checkbox"/> | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| 1.61 | | <input type="checkbox"/> | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| 4.10 | | <input type="checkbox"/> | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| 14.47 | | <input type="checkbox"/> | <input checked="" type="checkbox"/> | <input type="checkbox"/> |

Chromatograms

Item name: 310811_037
Channel name: Nefazodone+O [+H+]: (0.0200 Da) 486.2251

Spectra

Item name: 310811_037
Channel name: Low energy: Time 3.0713 +/- 0.0...
Description: Nefazodone T5, 10 x diluted with...

选择 Show all components for selected sample

View 选择 Metabolite Summary

View 选择 Show all components for selected sample

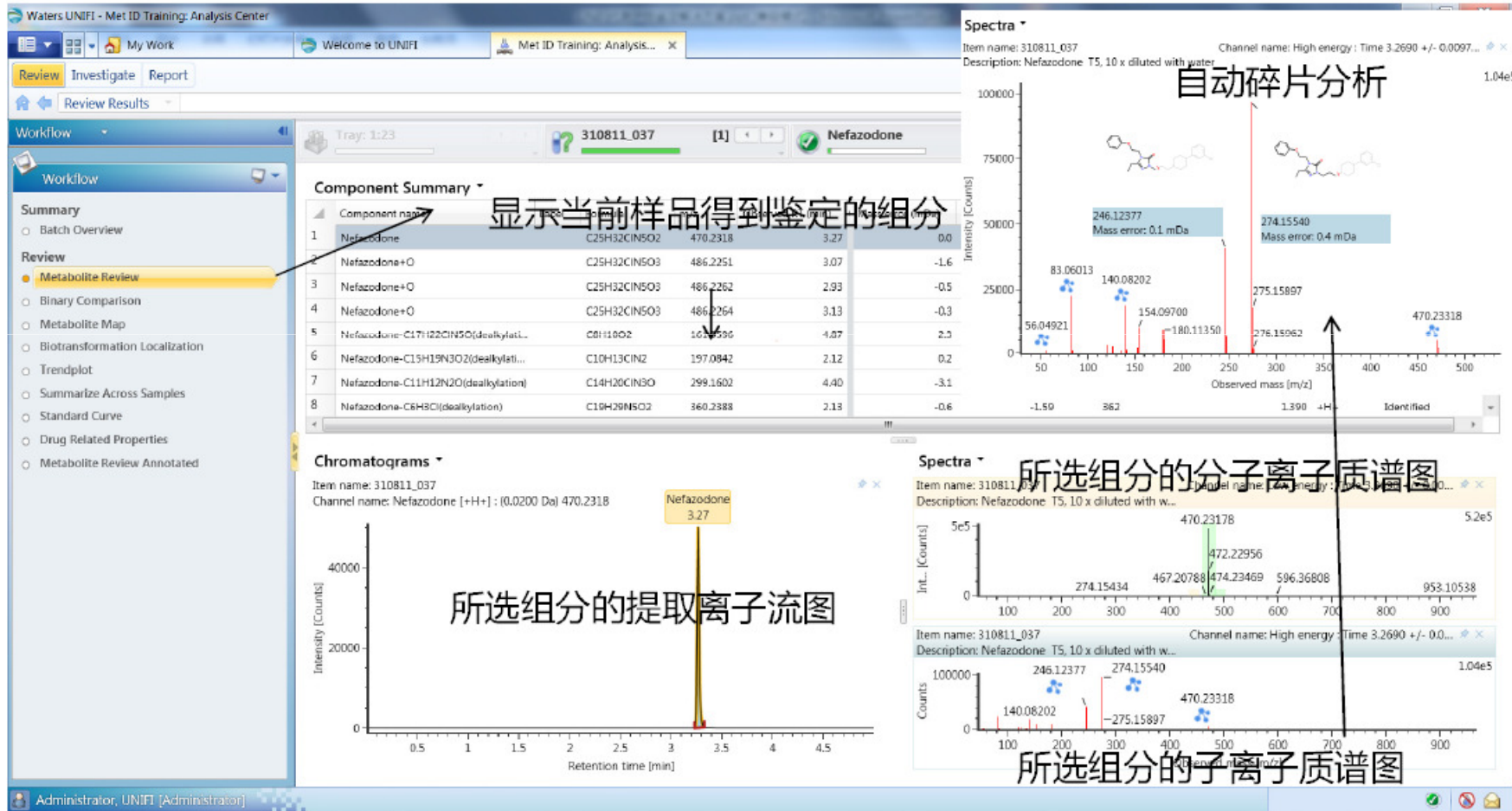
| Component name | Label | Formula | m/z | Observed RT (min) | Mass error (ppm) |
|---------------------------------------|-------|--------------|----------|-------------------|------------------|
| Nefazodone | | C25H32ClN5O2 | 470.2318 | 3.27 | |
| Nefazodone | | C25H32ClN5O2 | 470.2318 | 3.27 | |
| Nefazodone+O | | C25H32ClN5O3 | 486.2262 | 2.93 | |
| Nefazodone+O | | C25H32ClN5O3 | 486.2264 | 3.13 | |
| Nefazodone-C17H22ClN5O2(dealkylation) | | C8H10O2 | 161.0596 | 4.87 | |
| Nefazodone-C15H19N3O2(dealkylation) | | C10H13ClN2 | 197.0842 | 2.12 | |
| Nefazodone-C11H12N2Cl(dealkylation) | | C14H20ClN3O | 299.1602 | 4.40 | |
| Nefazodone-C6H9Cl(dealkylation) | | C10H20N5O2 | 360.2388 | 2.13 | |
| Nefazodone-C2H2(dealkylation) | | C23H30ClN5O2 | 444.2163 | 3.26 | |

Chromatograms

Item name: 310811_037
Channel name: Nefazodone [+H+] : (0.0200 Da) 470.2318

Spectra

Item name: 310811_037
Channel name: Low energy : Time 3.2690 +/- 0.0...
Description: Nefazodone T5, 10 x diluted with...



考察母药的裂解

Waters UNIFI - Met ID Training: Analysis Center

Workflow: 310811_037 [1] Nefazodone

Component Summary

| Component name | Label | Formula | m/z | Observed RT (min) | Mass error (mDa) | Mass error (ppm) | Response | Percentage of Parent Response (%) | Adducts | Identification status |
|---------------------------------------|-------|----------|-----------|-------------------|------------------|------------------|----------|-----------------------------------|------------|-----------------------|
| 1 Nefazodone | | C25H32O2 | 470.23178 | 3.27 | 0.0 | 0.10 | 26032 | 100.000 | +H+, +Na | Identified |
| 2 Nefazodone+O | | C25H32O3 | 472.22956 | 3.27 | -1.6 | -3.37 | 1853 | 7.143 | +H+ | Identified |
| 3 Nefazodone+O | | C25H32O3 | 474.23469 | 3.27 | -0.3 | -0.64 | 15 | 0.057 | +H+ | Identified |
| 4 Nefazodone+O | | C25H32O3 | 474.23469 | 3.27 | -0.3 | -0.67 | 46 | 0.175 | +H+ | Identified |
| 5 Nefazodone-C17H22ClN5O(alkylation) | | C8H10O2 | 141.052 | 2.3 | 2.3 | 14.56 | 24 | 0.091 | +Na | Identified |
| 6 Nefazodone-C15H15N3O2(dealkylation) | | C10H13O2 | 167.078 | 0.2 | 0.2 | 1.08 | 81 | 0.312 | +H+ | Identified |
| 7 Nefazodone-C11H12N2O(dealkylation) | | C14H20O2 | 228.144 | -3.1 | -10.52 | 26 | 0.099 | +NH4 | Identified | |
| 8 Nefazodone-C6H5Cl(dealkylation) | | C19H20N5 | 324.154 | -0.6 | -1.59 | 362 | 1.390 | +H+ | Identified | |
| 9 Nefazodone-C2H2(dealkylation) | | C23H30O2 | 368.222 | 0.2 | 0.2 | 0.44 | 49 | 0.187 | +H+ | Identified |

右键点击母药，选择Elucidate

Chromatograms

Item name: 310811_037
Channel name: Nefazodone [+H+]: (0.0200 Da) 470.2318

Spectra

Item name: 310811_037
Channel name: Low energy: Time 3.2690 +/- 0.00...
Description: Nefazodone T5, 10 x diluted with w...

Item name: 310811_037
Channel name: High energy: Time 3.2690 +/- 0.00...
Description: Nefazodone T5, 10 x diluted with w...

分析母离子（原药）的碎片信息

The screenshot displays the Waters UNIFI software interface. The main window shows two mass spectra for item 310811_037 (Nefazodone-T5...):

- Low energy spectrum:** X-axis is m/z (0-800), Y-axis is Intensity [Counts] (0-5.2e5). Major peaks are labeled at m/z 467.20788, 470.23178, 472.22956, 474.23469, and 953.10538.
- High energy spectrum:** X-axis is Observed mass [m/z] (0-800), Y-axis is Intensity [Counts] (0-1.04e5). Major peaks are labeled at m/z -275.15897, 274.15540, 470.23318, and 1.04e5.

A **Common Fragment Search** dropdown menu is open, listing various search methods. An arrow points to the **Fragment Match** option. The menu items include:

- Library Search
- ChemSpider Search
- Isotope Match
- Isotope Model
- Elemental Composition
- Fragment Match**
- Localize Transformation
- Halogen Match
- Neutral Loss
- Common Fragment Search
- Mass Defect Filter
- Manual Identification

Below the menu, a table shows search results:

| RT (min) | Match |
|----------|-------------------------------|
| 3.2690 | |
| 2 | Nefazodone-C2H2(dealkylation) |

The **Information** panel at the bottom shows a mass chromatogram with peaks at 3.266 and 3.206 minutes. The X-axis is Retention Time [min] (0-5), and the Y-axis is Intensity [Counts] (0-10000).

Text overlay: **Mass Fragment 匹配** (Mass Fragment Match)

分析母离子的碎片信息

选择离子化模式

碎片的理论 m/z

| Peak Id | Peak Mass (Da) | Mass (Da) | DBE | Mass Difference (mDa) | Formula | Formula Difference | Assignments | |
|---------|----------------|-----------|----------|-----------------------|---------|--|---|---|
| 1 | 4 | 126.0655 | 126.0662 | 3.5000 | -0.7 | C ₅ H ₈ N ₃ O ₁ | C ₂₀ H ₂₅ N ₂ O ₁ Cl ₁ | 5 |
| 2 | 6 | 140.0820 | 140.0818 | 3.5000 | 0.2 | C ₆ H ₁₀ N ₃ O ₁ | C ₁₉ H ₂₃ N ₂ O ₁ Cl ₁ | 5 |
| 3 | 8 | 153.0896 | 153.0897 | 4.0000 | 0.0 | C ₇ H ₁₁ N ₃ O ₁ | C ₁₈ H ₂₂ N ₂ O ₁ Cl ₁ | 4 |
| 4 | 9 | 154.0970 | 154.0975 | 3.5000 | -0.5 | C ₇ H ₁₂ N ₃ O ₁ | C ₁₈ H ₂₁ N ₂ O ₁ Cl ₁ | 4 |

Mass: 126.06619 DBE: 3.5 Mass Difference: -0.65793 Formula: C₅H₈N₃O₁ Formula Difference: C₂₀H₂₅N₂O₁Cl₁

中性丢失扫描，寻找具有相同中性丢失的化合物

Workflow

Summary

- Batch Overview
- Review
 - Metabolite Review
 - Elucidation Toolset**
 - Binary Comparison
 - Metabolite Map
 - Biotransformation Localization
 - Trendplot
 - Summarize Across Samples
 - Standard Curve
 - Drug Related Properties
 - Metabolite Review Annotated

Spectra

Item name: 310811_037 Channel name: Low energy : TL...
Description: Nefazodone T5... 5.2e5

Intensity [Counts]

470.23178
472.22956
467.20788 474.23469

Item name: 310811_037 Channel name: High energy ...
Description: Nefazodone T5... 1.04e5

Intensity [Counts]

274.15540
-275.15897
470.23318

Observed mass [m/z]

Neutral Loss

Parameters

Mass: 79.9568 Da
Formula: C5H7O3N
Tolerance: 10 mDa

Start

Results (0 found)

| Mass | Formula | Name |
|----------|---------|-------------------|
| 79.9568 | SO3 | Sulfate |
| 129.0426 | C5H7O3N | Pyroglutamic acid |
| 176.0321 | C6H8O6 | Glucuronide |

Filter Clear Filter

Information

输入常用的ESI+中性丢失的分子式

点击Start搜索所有的Components中具有相同中性丢失的组分

中性丢失扫描，寻找具有相同中性丢失的化合物

The screenshot displays the Waters UNIFI software interface. On the left, a 'Workflow' sidebar lists various analysis steps, with 'Elucidation Toolset' selected. The main area shows two mass spectra for item 310811_037 (Nefazodone). The top spectrum is a 'Low energy' scan with a base peak at m/z 470.23178 and other significant peaks at 472.22956, 467.20788, 474.23469, and 898.90719. The bottom spectrum is a 'High energy' scan with a base peak at m/z 274.15540 and another peak at 470.23318. On the right, a 'Neutral Loss' search menu is open, listing various search criteria such as Library Search, ChemSpider Search, Isotope Match, etc. The 'Neutral Loss' option is highlighted. A red arrow points from the Chinese text '选择Neutral Loss' to the 'Neutral Loss' menu item. Below the menu, there are 'Filter' and 'Clear Filter' buttons. The bottom status bar shows 'Administrator, UNIFI [Administrator]'.

子离子扫描，寻找具有相同子离子的化合物

The screenshot displays the Waters UNIFI software interface. The main window shows two mass spectra for item 310811_037 (Nefazodone). The top spectrum is labeled 'Low energy : TL' with a scale of 5.2e5. The bottom spectrum is labeled 'High energy ...' with a scale of 1.04e5. A search menu is open over the 'Neutral Loss' section, with 'Common Fragment Search' highlighted. A handwritten Chinese annotation '选择Common Fragment Search' with an arrow points to this option. The interface includes a 'Workflow' sidebar on the left, a top navigation bar with 'Review', 'Investigate', and 'Report' tabs, and a status bar at the bottom.

Spectra

Item name: 310811_037 Channel name: Low energy : TL
Description: Nefazodone TS... 5.2e5

| Observed mass [m/z] | Intensity [Counts] |
|---------------------|--------------------|
| 467.20788 | ~1e5 |
| 470.23178 | ~4e5 |
| 472.22956 | ~2e5 |
| 474.23469 | ~1e5 |
| 898.90719 | ~1e5 |

Item name: 310811_037 Channel name: High energy ...
Description: Nefazodone TS... 1.04e5

| Observed mass [m/z] | Intensity [Counts] |
|---------------------|--------------------|
| -275.15897 | ~100000 |
| 274.15540 | ~100000 |
| 470.23318 | ~10000 |

Neutral Loss

- Library Search
- ChemSpider Search
- Isotope Match
- Isotope Model
- Elemental Composition
- Fragment Match
- Localize Transformation
- Halogen Match
- Neutral Loss
- Common Fragment Search**
- Mass Defect Filter
- Manual Identification

选择Common Fragment Search

子离子扫描，寻找具有相同子离子的化合物

Waters UNIFI - Met ID Training: Analysis Center

Workflow: 310811_037 [1] Nefazodone

Spectra
Item name: 310811_037 Channel name: Low energy : TL...
Description: Nefazodone T5...
Intensity [Counts] vs Observed mass [m/z]. Peaks at 274.15434 and 444.21627.

Common Fragment Search
Parameters:
Fragment Mass: 274.1554 Da
Mass Tolerance: 10 mDa
Start
Results (2 found):

| Component Name | RT (min) |
|---------------------------------|----------|
| 1 Nefazodone | 3.2690 |
| 2 Nefazodone-C2H2(dealkylation) | 3.2650 |

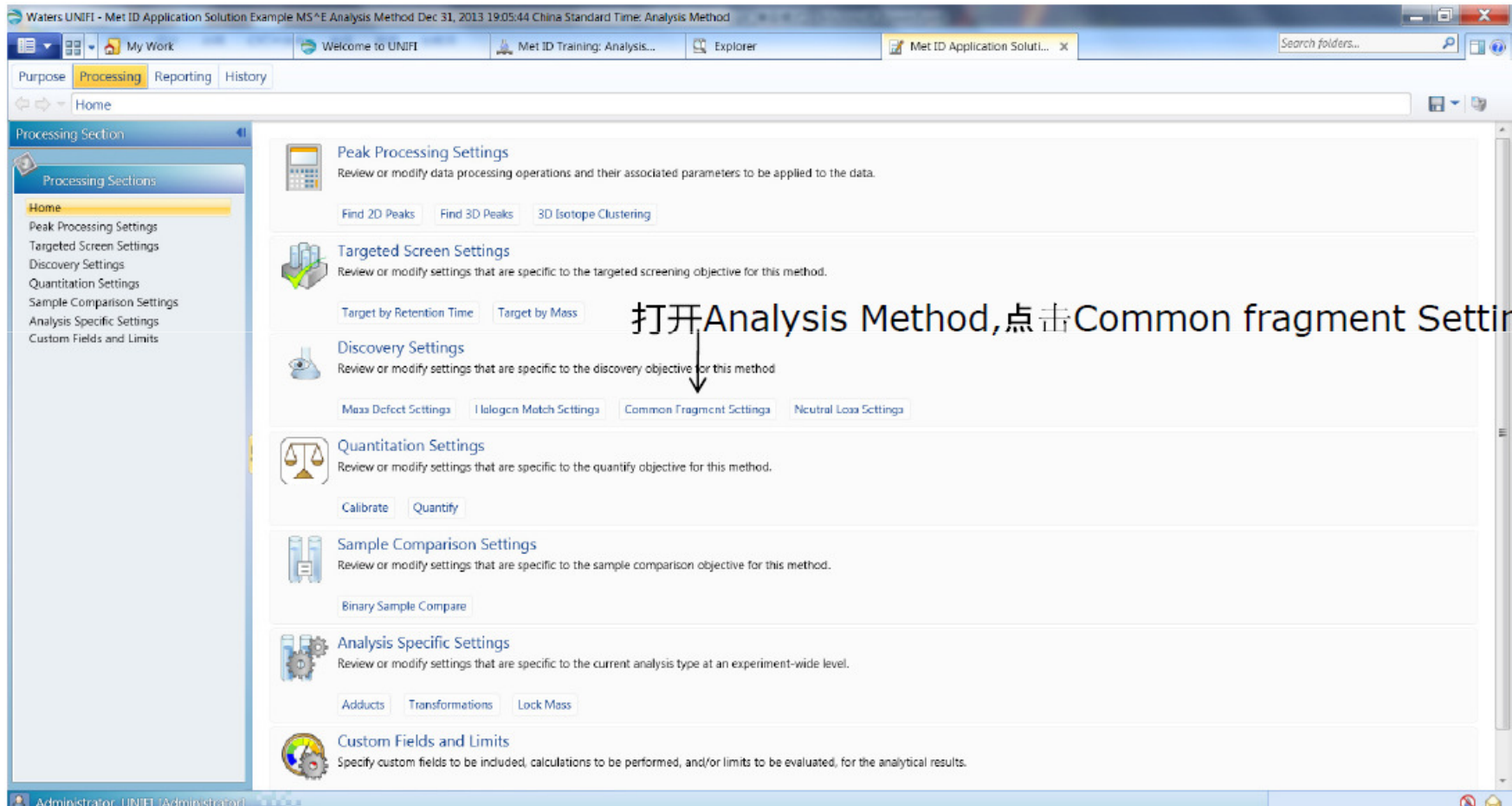
Information
Mass Chromatogram (0.0100 Da) :-83.0601 : 2: TOF MSe (50-1200) 0eV ESI+
Intensity [Counts] vs Retention Time [min]. Peaks at 0.190, 2.130, 3.269, 3.284, 3.286, 3.328.

左键点击相应的子离子

点击Start搜索具有相同子离子的组分

子离子提取色谱图

可以将得到的母离子碎片信息添加到方法中



设置子离子丢失

注意选中

| | Mass |
|---|-----------|
| 1 | 56.04920 |
| 2 | 83.06040 |
| 3 | 140.08180 |
| 4 | 180.11310 |
| 5 | 246.12370 |
| 6 | 274.1550 |

可以把分析中发现的母药得到确证的, 强度比较大的子离子理论质量输入方法中

设置中性丢失

注意选中

保存后可以重新处理数据

同样也可以把常见的中性丢失分子式输入处理方法

| | Mass | Formula |
|---|------------|---------|
| 1 | 79.95681 | SO3 |
| 2 | 129.042... | C5H7O3N |
| 3 | 176.032... | C6H8O6 |

浏览二元比较结果

The screenshot displays the Waters UNIFI software interface for a binary comparison analysis. The main window shows the 'Component Summary' table, which compares an unknown component (Nefazodone+O) against a reference component (Nefazodone). The table includes columns for Label, Unknown component name, Reference component name, Match type, and various mass and retention time parameters.

| Label | Unknown component name | Reference component name | Match type | Unknown mass [Da] | Reference mass [Da] | Retention time [min] | Reference retention time [min] |
|-------|------------------------|--------------------------|----------------|-------------------|---------------------|----------------------|--------------------------------|
| 1 | Nefazodone | Nefazodone | Common | 470.232 | 470.232 | 3.27 | 3.27 |
| 2 | Nefazodone+O | | Unknown Unique | 486.225 | 0.000 | 3.07 | 0.00 |
| 3 | Nefazodone+O | | Unknown Unique | 486.226 | 0.000 | 2.93 | 0.00 |
| 4 | Nefazodone+O | | Unknown Unique | 486.226 | 0.000 | 2.93 | 0.00 |

Annotations on the screenshot:

- An arrow points to the 'Common' match type in the table, with the text: "Common 表示Reference和Unknown共有的组分".
- An arrow points to the 'Unknown Unique' match types, with the text: "Unknown Unique 表示Unknown独有的组分".
- An arrow points to the 'Binary Comparison' option in the left-hand 'Review' menu, with the text: "点击Binary Compare".

The 'Chromatograms' section shows a single peak at 3.07 minutes for the Nefazodone+O component. The 'Spectra' section shows the mass spectrum for the Nefazodone+O component, with a base peak at 486.22506 m/z and other significant peaks at 487.22801, 488.22368, 489.22317, and 490.22444 m/z.

Metabolite map

Waters UNIFI - Met ID Application Solution Example MSⁿE Analysis Method Dec 31, 2013 19:05:44 China Standard Time Dec 31, 2013 22:49:36 China Standard Time: Analysis Center

My Work Welcome to UNIFI Met ID Application Soluti... x Search folders...

Review Investigate Report

Review Results

Limits Process Edit Tools File

Workflow Tray: 1:23 310811_037 [1] Nefazodone Filters

Workflow

- Summary
 - Batch Overview
- Review
 - Metabolite Review
 - Binary Comparison
 - Metabolite Map**
 - Biotransformation Localization
 - Trendplot
 - Summarize Across Samples
 - Standard Curve
 - Drug Related Properties
 - Metabolite Review Annotated

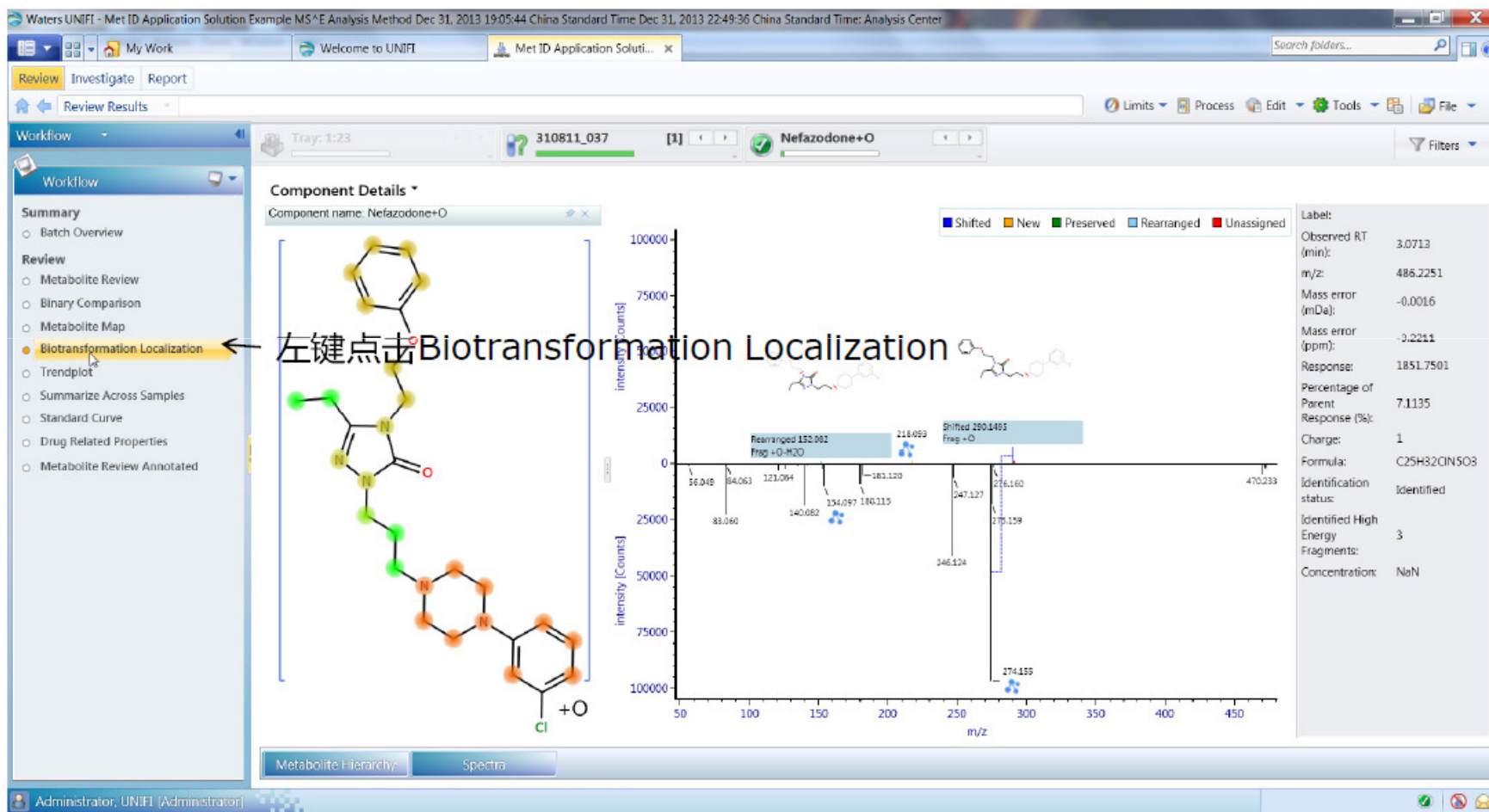
Metabolite Hierarchy

左键点击Metabolite Map

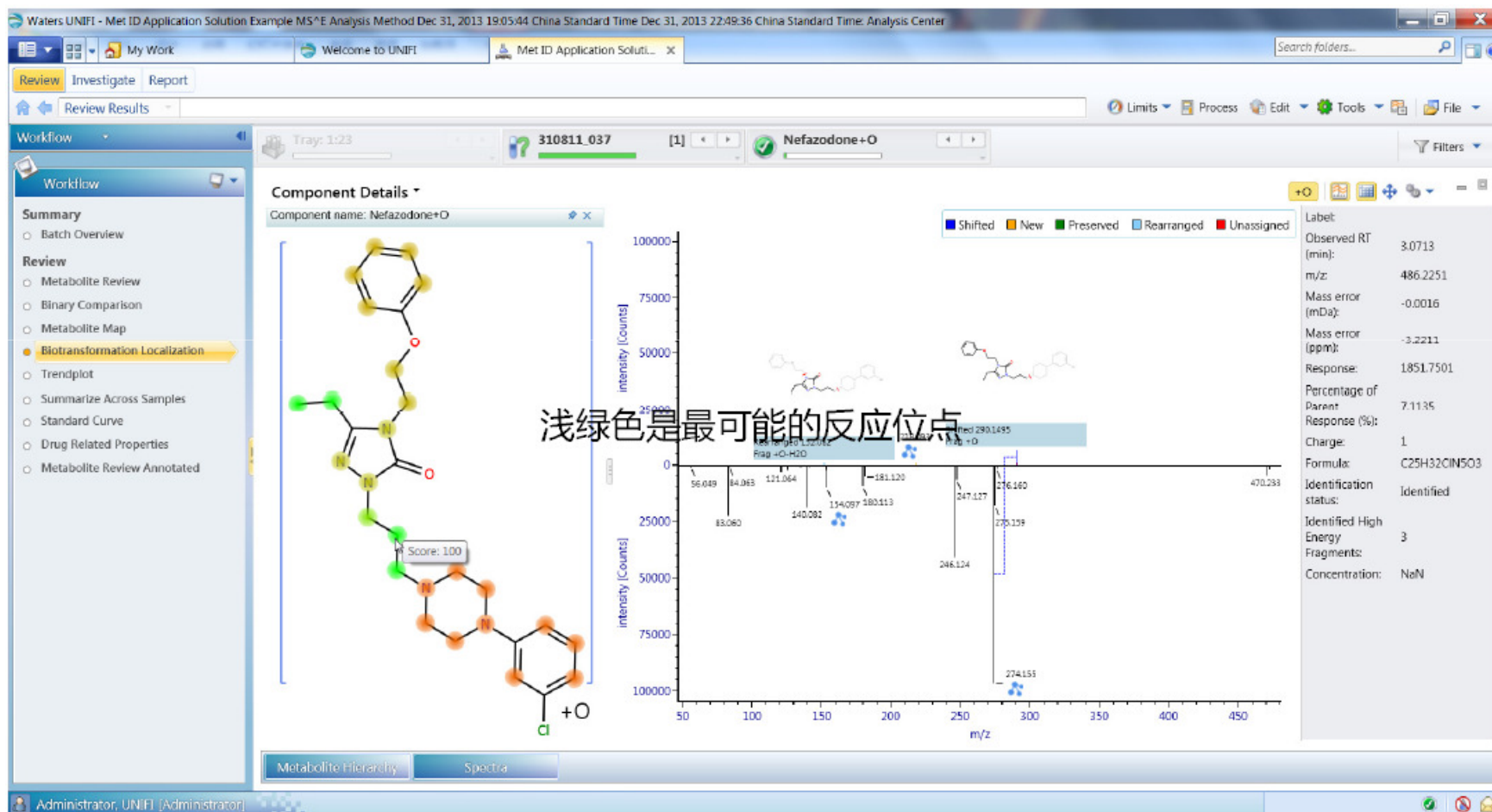
Component Summary Spectra

Administrator, UNIFI [Administrator]

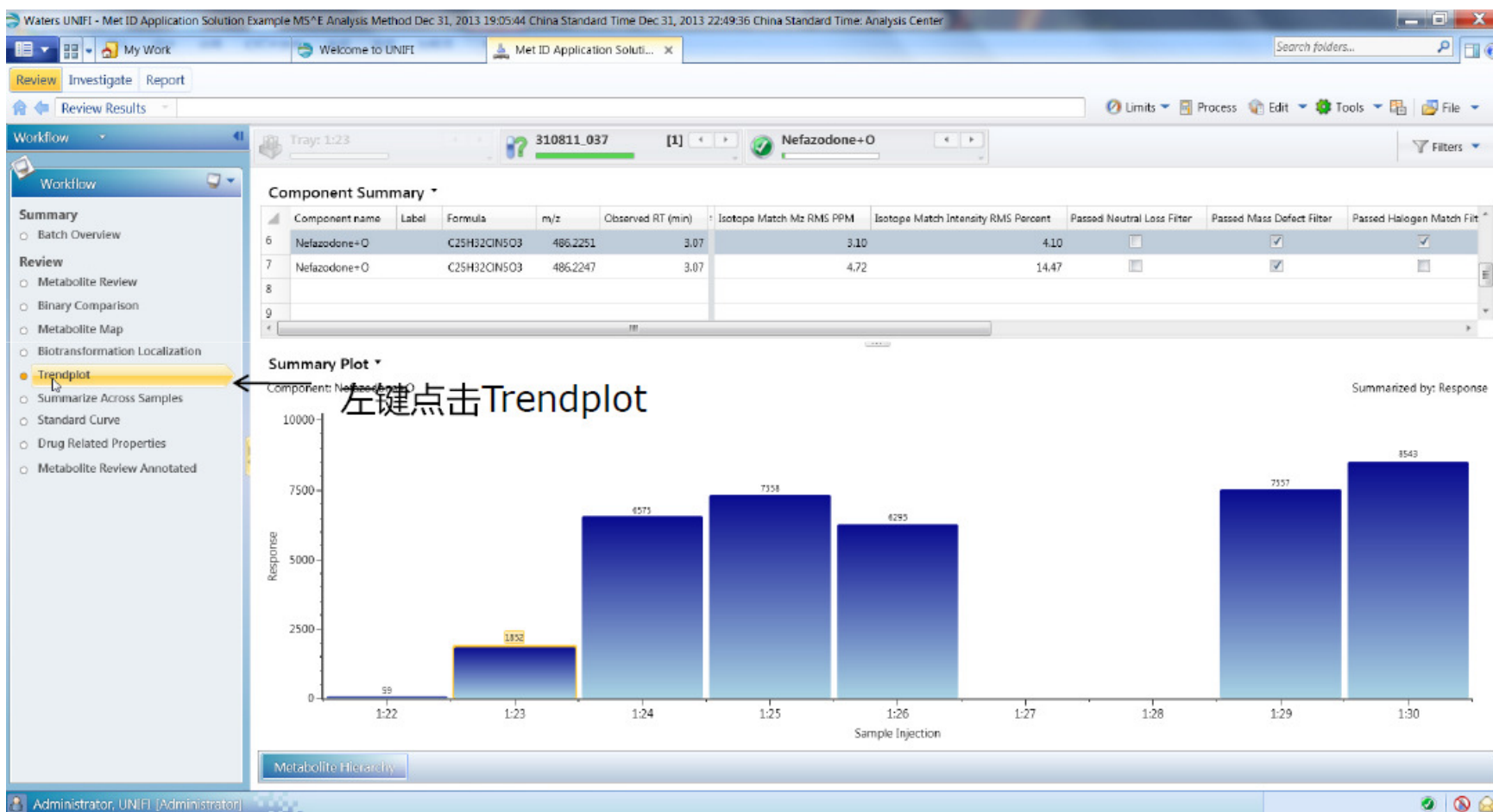
代谢位点



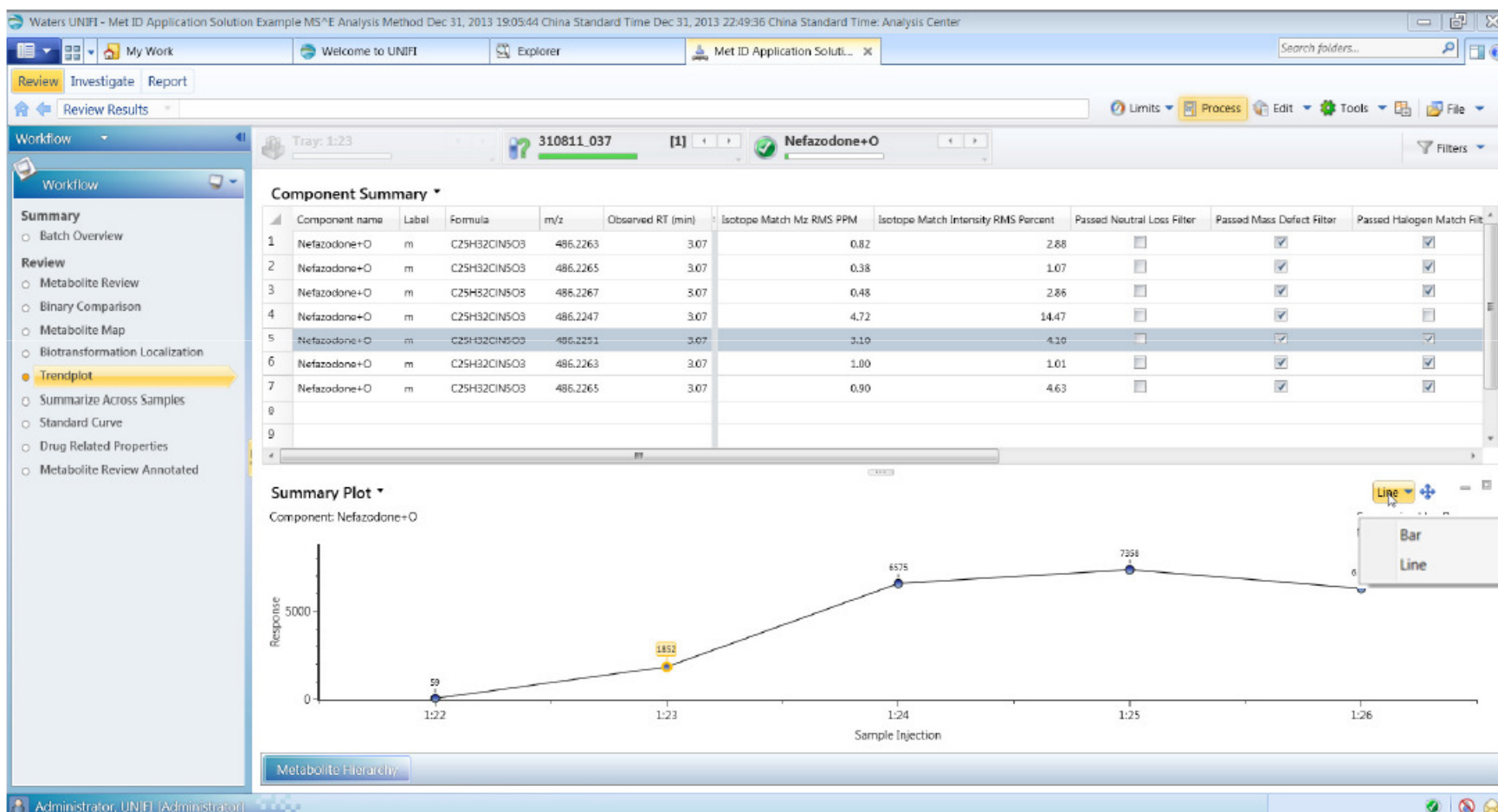
代谢位点



强度趋势图



强度趋势图



考察某一代谢物在所有样品中的情况

The screenshot displays the Waters UNIFI software interface. The main window shows a 'Component Summary' table for the metabolite 'Nefazodone+O'. The table lists 9 items with their respective replicate numbers and sample positions, along with various peak area values. A red arrow points to the 'Summarize Across Samples' option in the left-hand menu.

| Item name | Replicate number | Sample position | Nefazodone | Nefazodone+O | Nefazodone-C11H12N2O(deacetylation) | Nefazodone+O | Nefazodone+O | Nefazodone-C17H22CIN5O(deacetylation)+O | Nefazodone-C15H19N3O |
|-----------|------------------|-----------------|------------|--------------|-------------------------------------|--------------|--------------|---|----------------------|
| 1 | 310811_036 | 1 1:22 | 26192 | 59 | | 30 | | | |
| 2 | 310811_037 | 1 1:23 | 26032 | 1852 | | 26 | 141 | 46 | 24 |
| 3 | 310811_038 | 1 1:24 | 21988 | 6575 | | 31 | 409 | | |
| 4 | 310811_039 | 1 1:25 | 15884 | 7358 | | | 357 | | 30 |
| 5 | 310811_040 | 1 1:26 | 12105 | 6293 | | | 148 | | |
| 6 | 310811_041 | 1 1:27 | 23974 | | | | | | 35 |
| 7 | 310811_042 | 1 1:28 | 33447 | | | | | | 25 |
| 8 | 310811_043 | 1 1:29 | 16084 | 7177 | | 42 | | | |
| 9 | 310811_044 | 1 1:30 | 17588 | 8543 | | | | | |

代谢产物与原药的相关性

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Workflow: Tray: 1:23, 310811_037 [1], Candidate Mass 274...

Component Summary

| Component name | Label | Formula | m/z | Observed RT (min) | Passed Neutral Loss Filter | Passed Mass Defect Filter | Passed Halogen Match Filter | Passed Fragment Search F... | Ident |
|----------------|---|--|----------|-------------------|----------------------------|-------------------------------------|-------------------------------------|-------------------------------------|-------|
| 154 | Candidate Mass 204.0872 | | 204.0872 | 4.84 | <input type="checkbox"/> | <input checked="" type="checkbox"/> | <input type="checkbox"/> | <input type="checkbox"/> | |
| 155 | Candidate Mass 116.0527 | | 116.0527 | 4.84 | <input type="checkbox"/> | <input checked="" type="checkbox"/> | <input type="checkbox"/> | <input type="checkbox"/> | |
| 156 | Candidate Mass 415.0422 | | 415.0422 | 4.84 | <input type="checkbox"/> | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> | <input type="checkbox"/> | |
| 157 | Candidate Mass 88.0219 | | 88.0219 | 4.84 | <input type="checkbox"/> | <input checked="" type="checkbox"/> | <input type="checkbox"/> | <input type="checkbox"/> | |
| 158 | Candidate Mass 471.1042 | | 471.1042 | 4.84 | <input type="checkbox"/> | <input type="checkbox"/> | <input checked="" type="checkbox"/> | <input type="checkbox"/> | |
| 159 | Candidate Mass 144.9824 | | 144.9824 | 4.87 | <input type="checkbox"/> | <input checked="" type="checkbox"/> | <input type="checkbox"/> | <input type="checkbox"/> | |
| 160 | Candidate Mass 432.9946 | | 432.9946 | 4.96 | <input type="checkbox"/> | <input type="checkbox"/> | <input checked="" type="checkbox"/> | <input type="checkbox"/> | |
| 161 | Candidate Mass 173.1160 | | 173.1160 | 4.98 | <input type="checkbox"/> | <input checked="" type="checkbox"/> | <input type="checkbox"/> | <input type="checkbox"/> | |
| 162 | Candidate Mass 423.1543 | | 423.1543 | 4.98 | <input type="checkbox"/> | <input checked="" type="checkbox"/> | <input type="checkbox"/> | <input type="checkbox"/> | |
| 163 | Candidate Mass 118.0543 | | 118.0543 | 4.98 | <input type="checkbox"/> | <input checked="" type="checkbox"/> | <input type="checkbox"/> | <input type="checkbox"/> | |
| 164 | Candidate Mass 57.0698 | | 57.0698 | 4.98 | <input type="checkbox"/> | <input checked="" type="checkbox"/> | <input type="checkbox"/> | <input type="checkbox"/> | |
| 165 | Candidate Mass 133.0868 | | 133.0868 | 4.98 | <input type="checkbox"/> | <input checked="" type="checkbox"/> | <input type="checkbox"/> | <input type="checkbox"/> | |
| 166 | Candidate Mass 371.1599 | | 371.1599 | 4.99 | <input type="checkbox"/> | <input checked="" type="checkbox"/> | <input type="checkbox"/> | <input type="checkbox"/> | |
| 167 | Nefazodone | C ₂₅ H ₃₂ O ₂ | 470.2318 | 3.27 | <input type="checkbox"/> | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> | |
| 168 | Nefazodone-C ₂ H ₂ (dealkylation) | C ₂₃ H ₃₀ O ₂ | 444.2163 | 3.26 | <input type="checkbox"/> | <input checked="" type="checkbox"/> | <input type="checkbox"/> | <input checked="" type="checkbox"/> | |
| 169 | Candidate Mass 596.3681 | | 596.3681 | 3.27 | <input type="checkbox"/> | <input type="checkbox"/> | <input type="checkbox"/> | <input checked="" type="checkbox"/> | |
| 170 | Candidate Mass 470.3609 | | 470.3609 | 3.27 | <input type="checkbox"/> | <input type="checkbox"/> | <input type="checkbox"/> | <input checked="" type="checkbox"/> | |
| 171 | Candidate Mass 467.2079 | | 467.2079 | 3.27 | <input type="checkbox"/> | <input checked="" type="checkbox"/> | <input type="checkbox"/> | <input checked="" type="checkbox"/> | |
| 172 | Candidate Mass 274.1543 | | 274.1543 | 3.27 | <input type="checkbox"/> | <input checked="" type="checkbox"/> | <input type="checkbox"/> | <input checked="" type="checkbox"/> | |
| 173 | Candidate Mass 953.1054 | | 953.1054 | 3.27 | <input type="checkbox"/> | <input type="checkbox"/> | <input type="checkbox"/> | <input checked="" type="checkbox"/> | |

Workflow: Summary, Review, Drug Related Properties, Metabolite Review Annotated

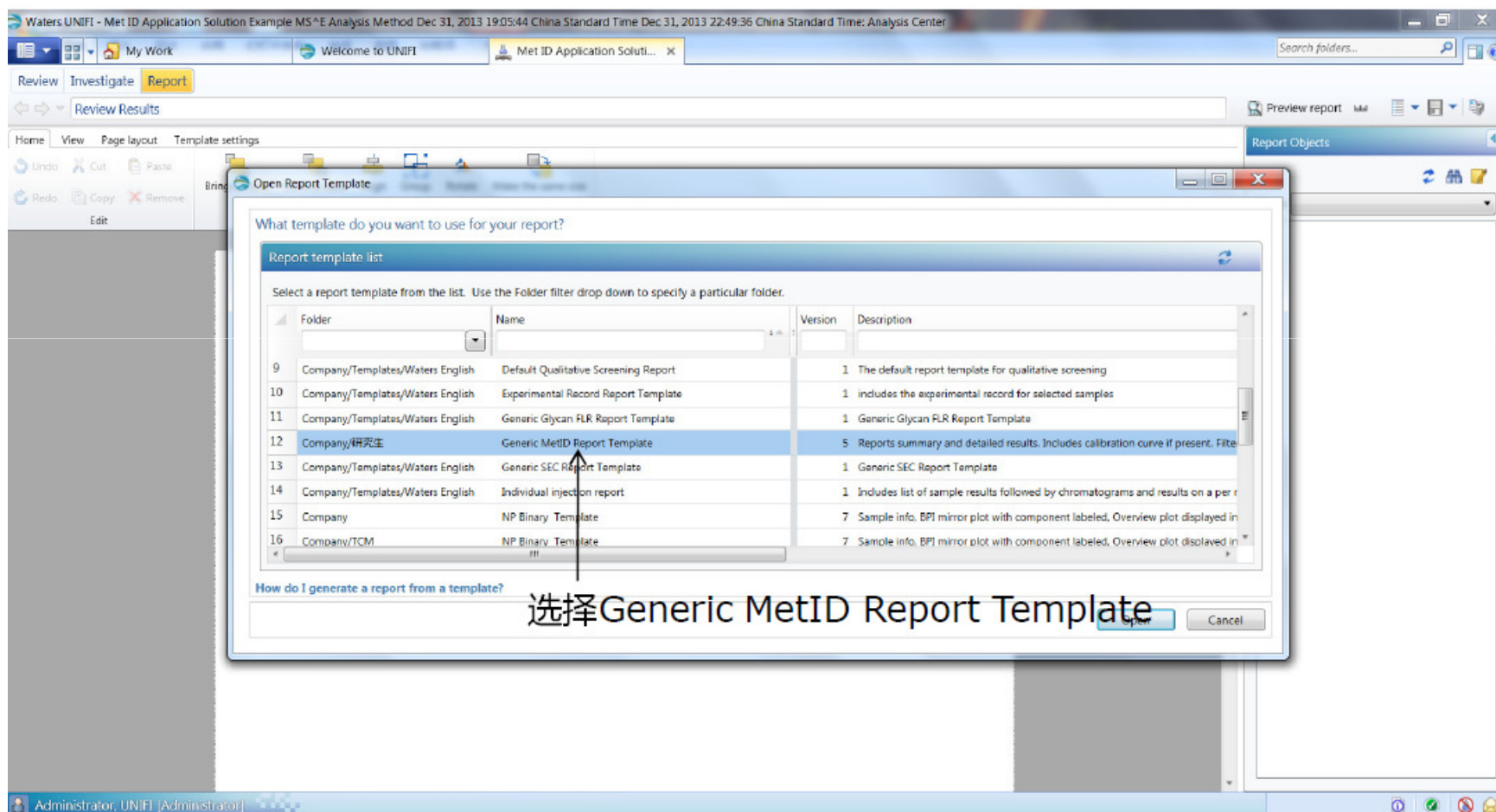
Chromatograms, Spectra

Administrator, UNIFI (Administrator)

左键点击 Drug Related Properties

上面任何一项通过的都可能是代谢产物；
除此之外，还需要考虑Binary Compare的结果

选择报告模板



预览报告



预览报告

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My Work Welcome to UNIFI Met ID Application Soluti...

Review Investigate **Report**

Review Results Preview Report Modify template File

Pages

Home Signature

Report 1 of 82 100% Rotate Find Selection mode Graphic Manage

Print Page Zoom Layout Search Copy Extract Export Apply

Reuse Extraction method

Waters
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UNIFI

Analysis Information

Item name: Met ID Application Solution Example MSⁿE Analysis Method Dec 31, 2013 19:05:44 China Standard Time Dec 31, 2013 22:49:36 China Standard Time Modified date:

Sample Set Instrument system name: SYNAPT-G2#NotSet Modified by:

Analysis Method Report

Purpose

| | |
|--|--|
| Item name: Met ID Application Solution Example MS ⁿ E Analysis Method Dec 31, 2013 19:05:44 China Standard Time | Quantify enabled: Yes |
| Description: Generic method to process Met ID data with Standards, Reference (t0) and Unknowns (t1..tn) | Compare enabled: Yes |
| Instrument system type: | Discover enabled: Yes |
| Analysis type: Metabolite Identification - MS ⁿ E | Matrix Factor Enabled: No |
| Analysis type description: Metabolite Identification on MS ⁿ E data | Separation enabled: No |
| Accurate mass: Accurate mass | Analyte class: SmallMolecule |
| Screen enabled: Yes | Analyte class description: SmallMolecule |
| | Analyte: |

Results not

Administrator, UNIFI [Administrator]

储存报告为PDF格式

