PeakView软件手动拟合化学式

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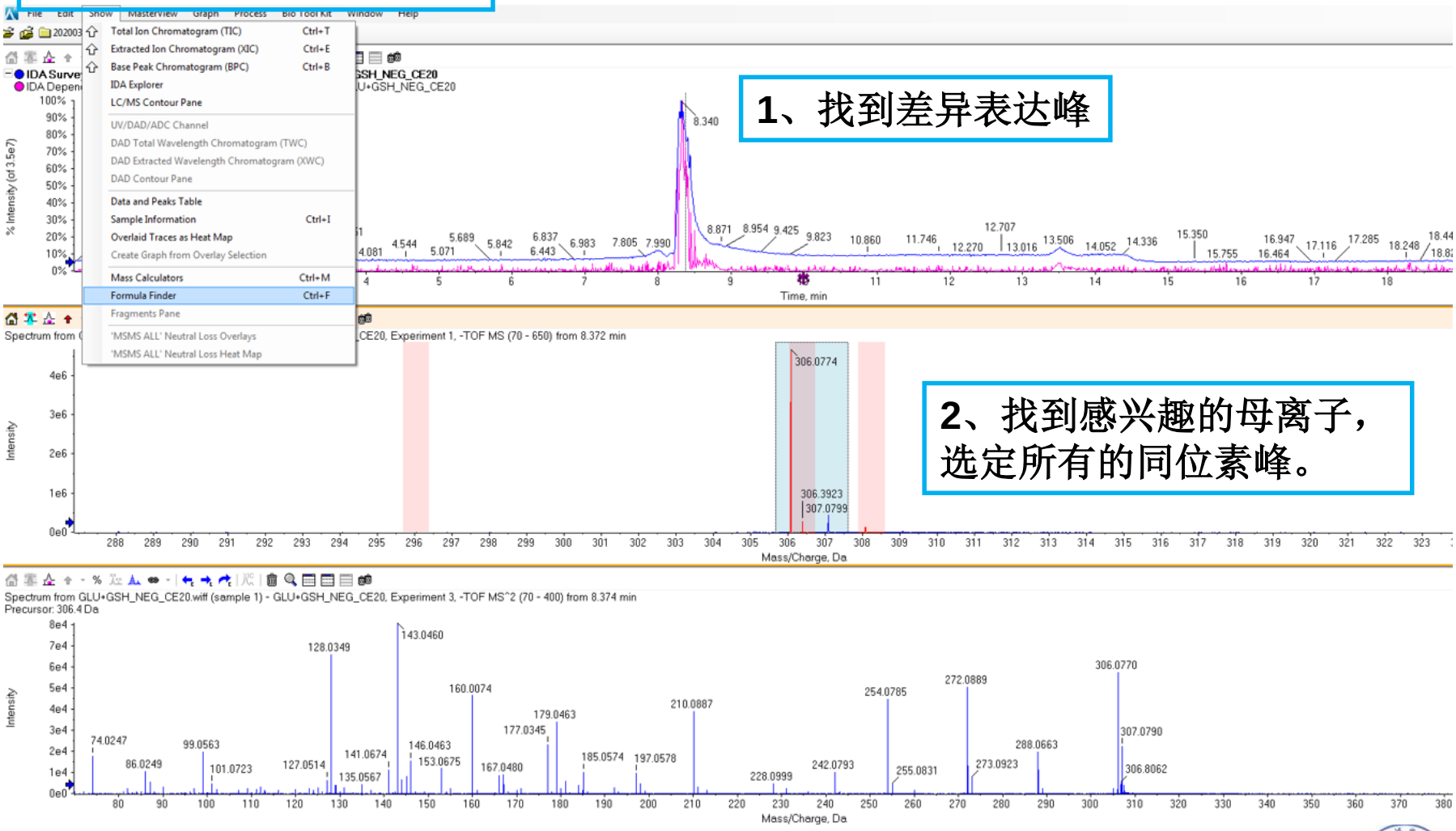
打开一个数据

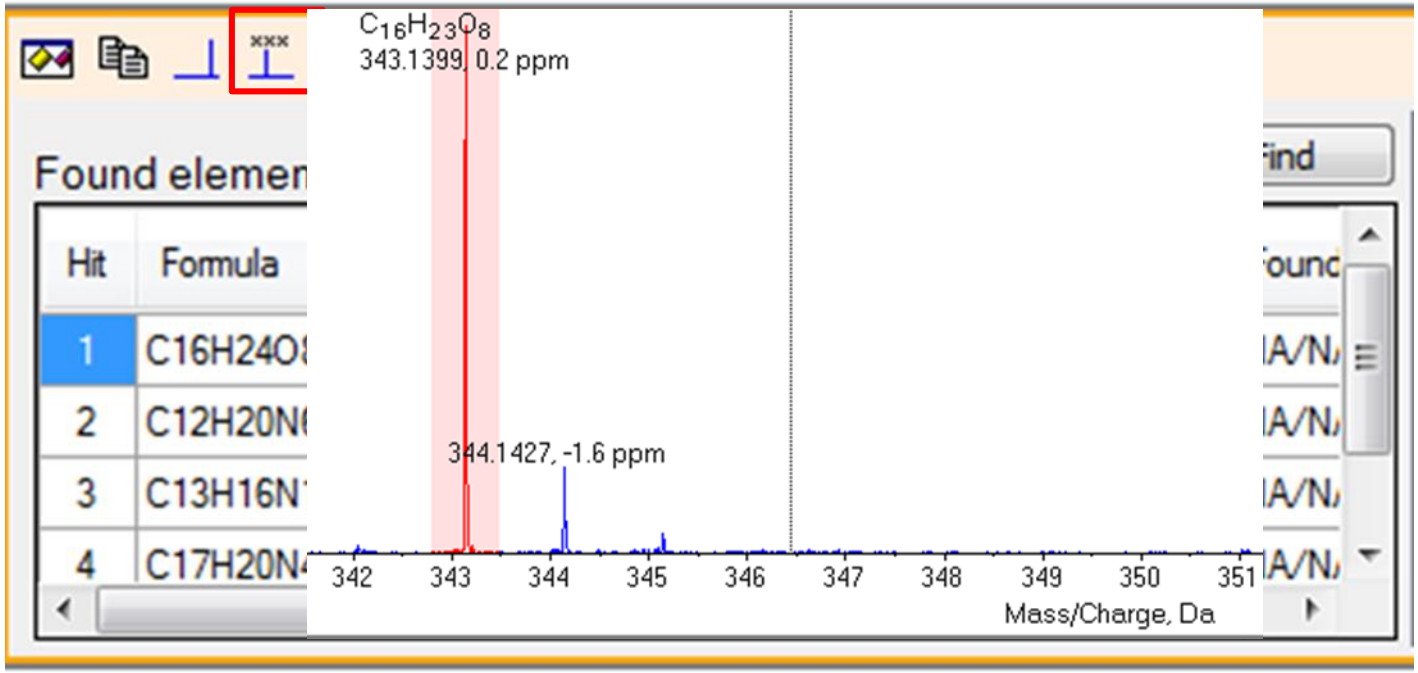
3、Show-formula finder



1、找到差异表达峰

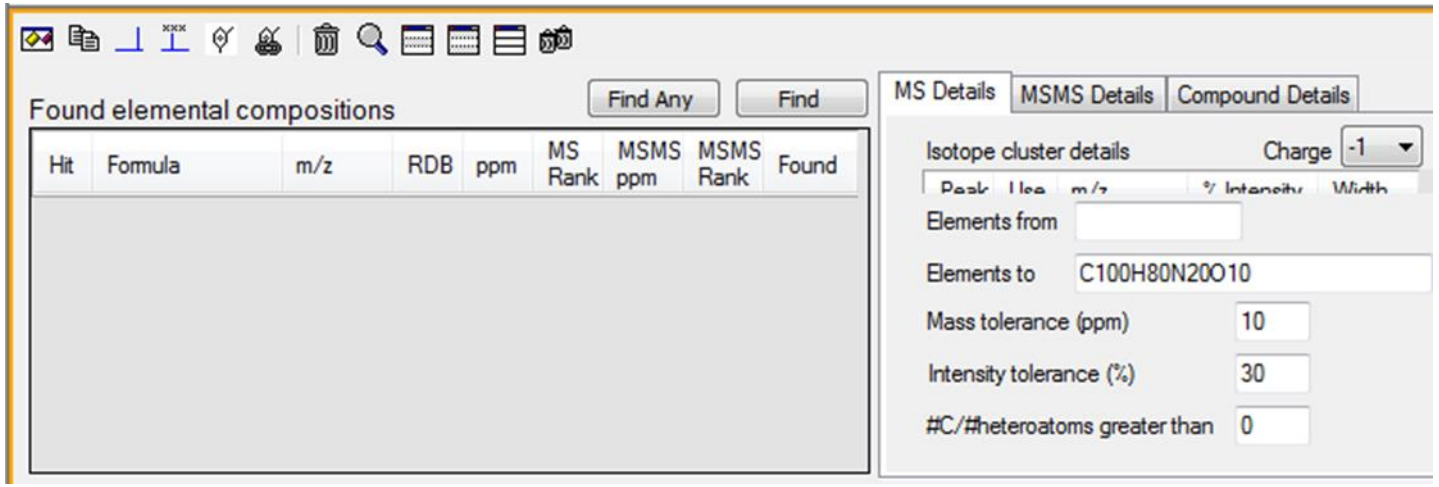
2、找到感兴趣的母离子，选定所有的同位素峰。

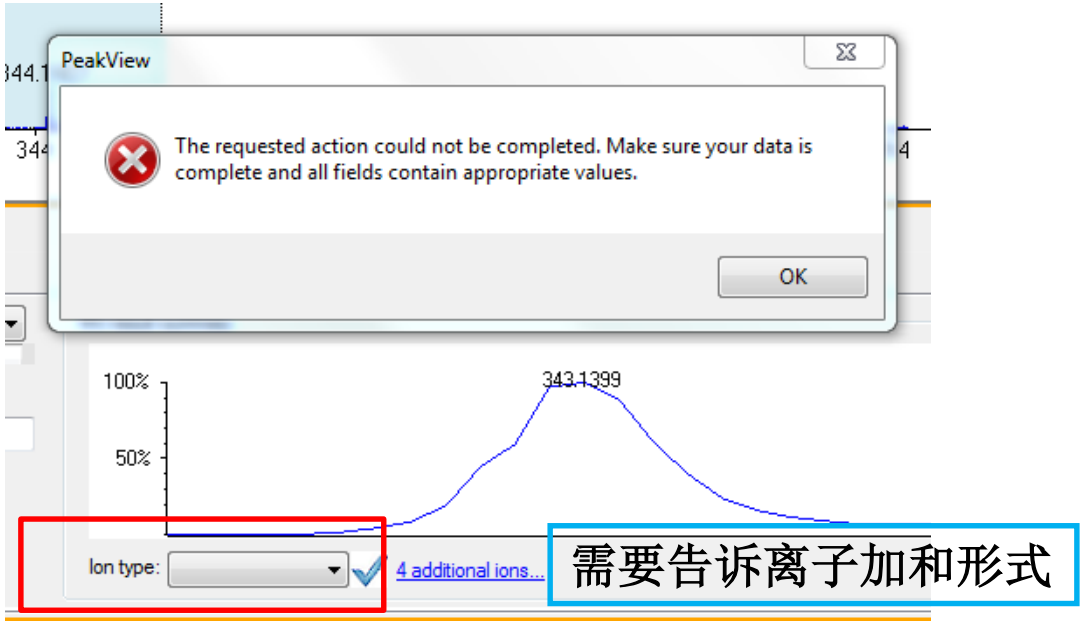
拟合结果



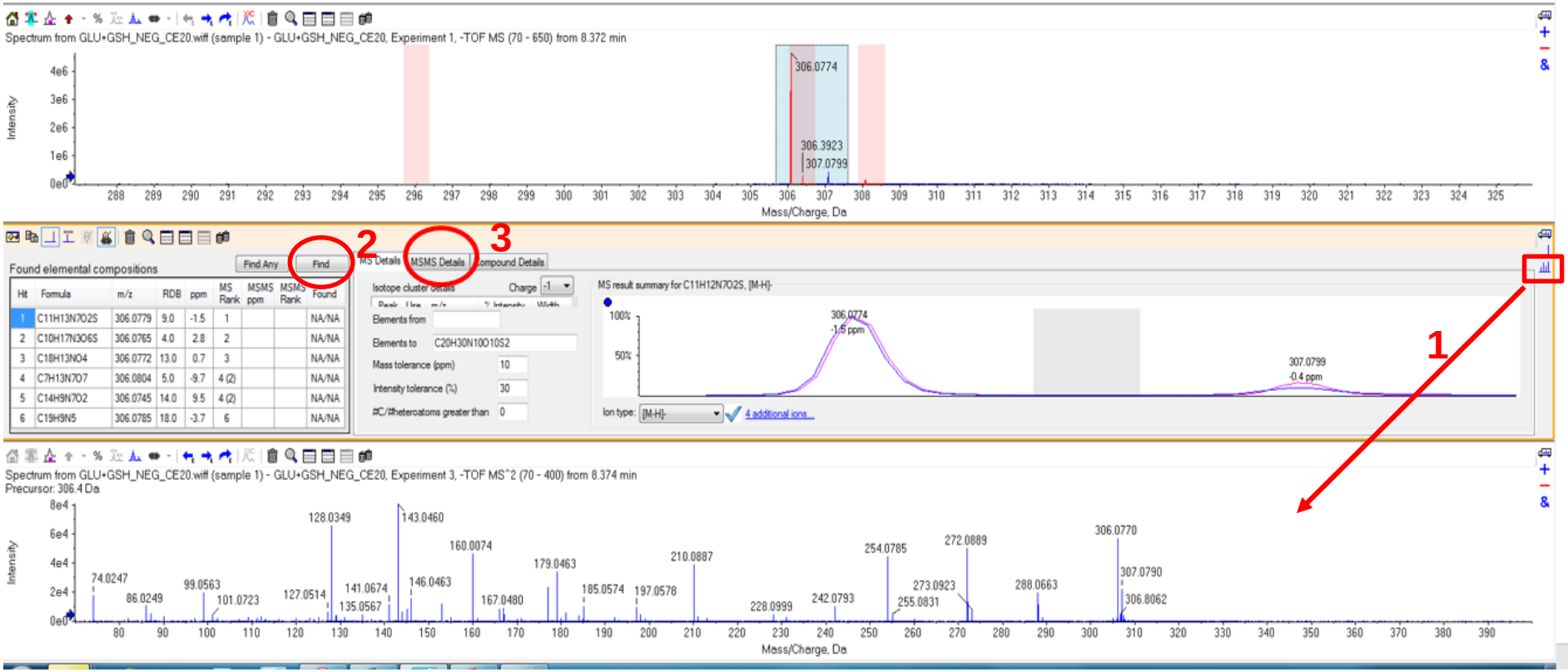
点击红色图标，可在一级质谱上标记选中的**fomula**及**error**

拟合无结果


Found elemental compositions
Find Any
Find
Hit
Formula
m/z
RDB
ppm
MS Rank
MSMS ppm
MSMS Rank
Found
MS Details
MSMS Details
Compound Details
Isotope cluster details
Charge
-1
Elements from
Elements to
C100H80N20O10
Mass tolerance (ppm)
10
Intensity tolerance (%)
30
#C/#heteroatoms greater than
0

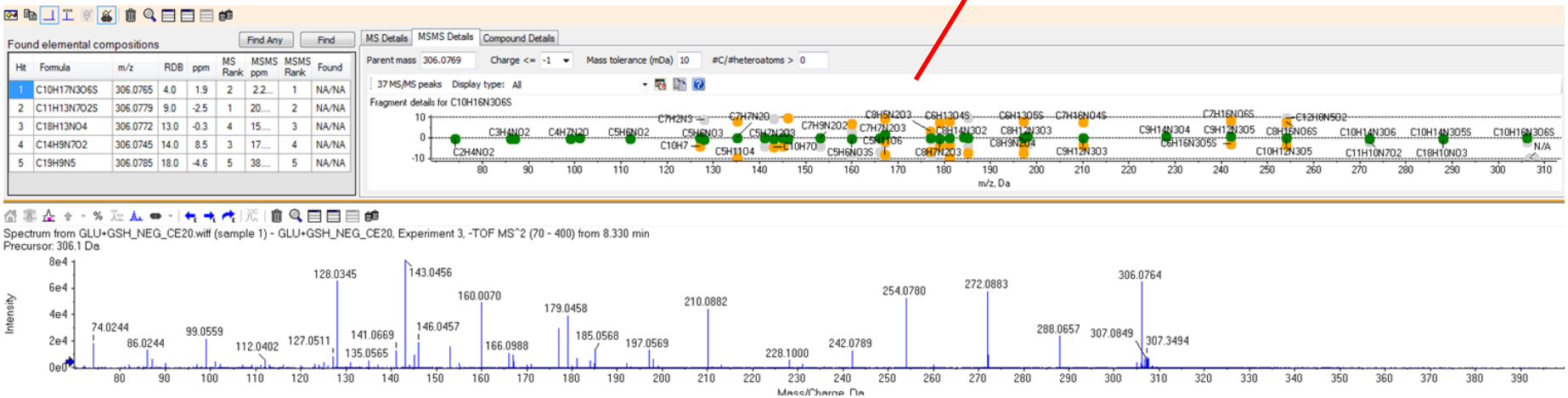

PeakView
The requested action could not be completed. Make sure your data is complete and all fields contain appropriate values.
OK
100%
50%
343.1399
Ion type:
4 additional ions...
需要告诉离子加和形式

匹配理论和实测二级

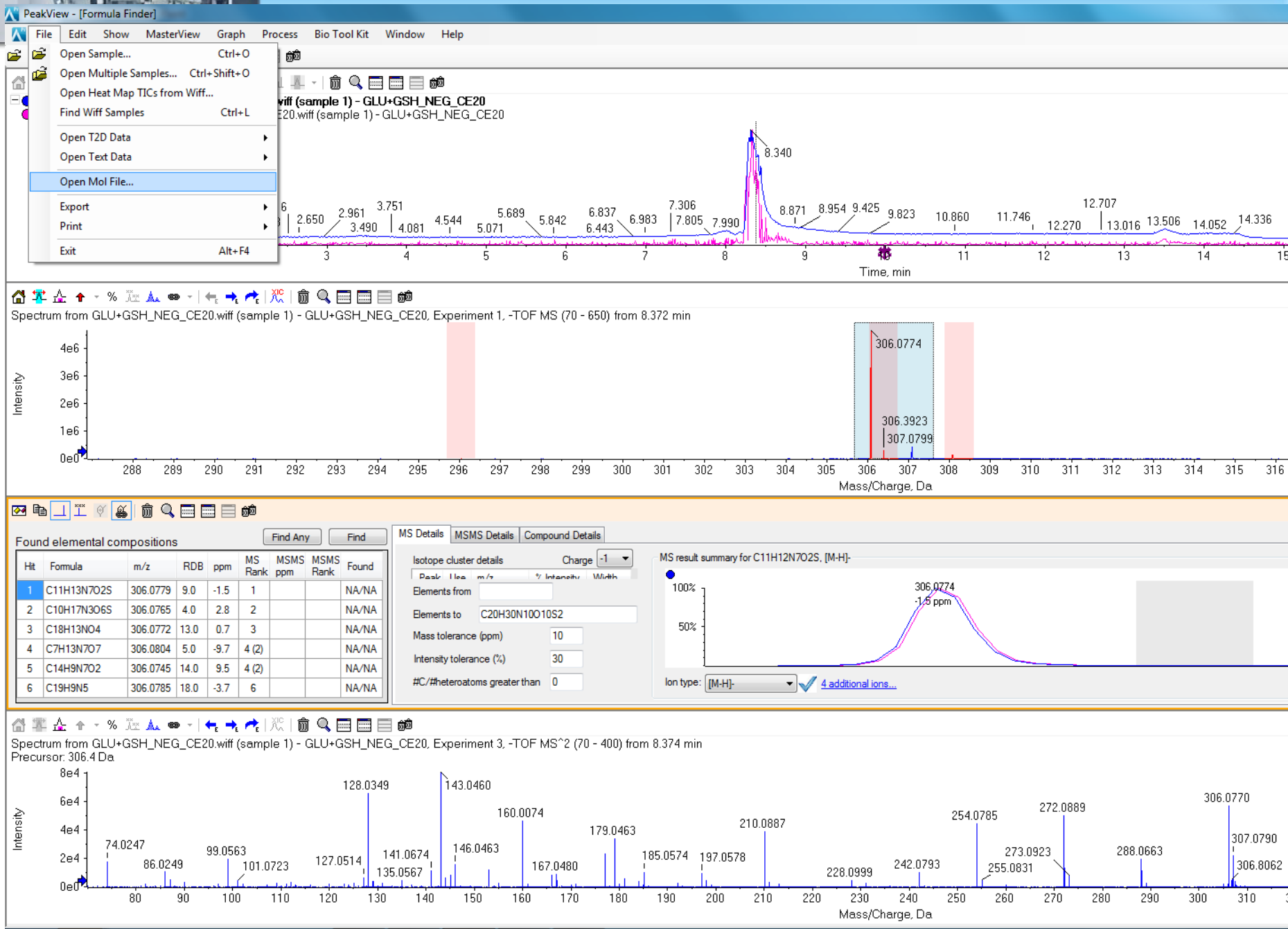


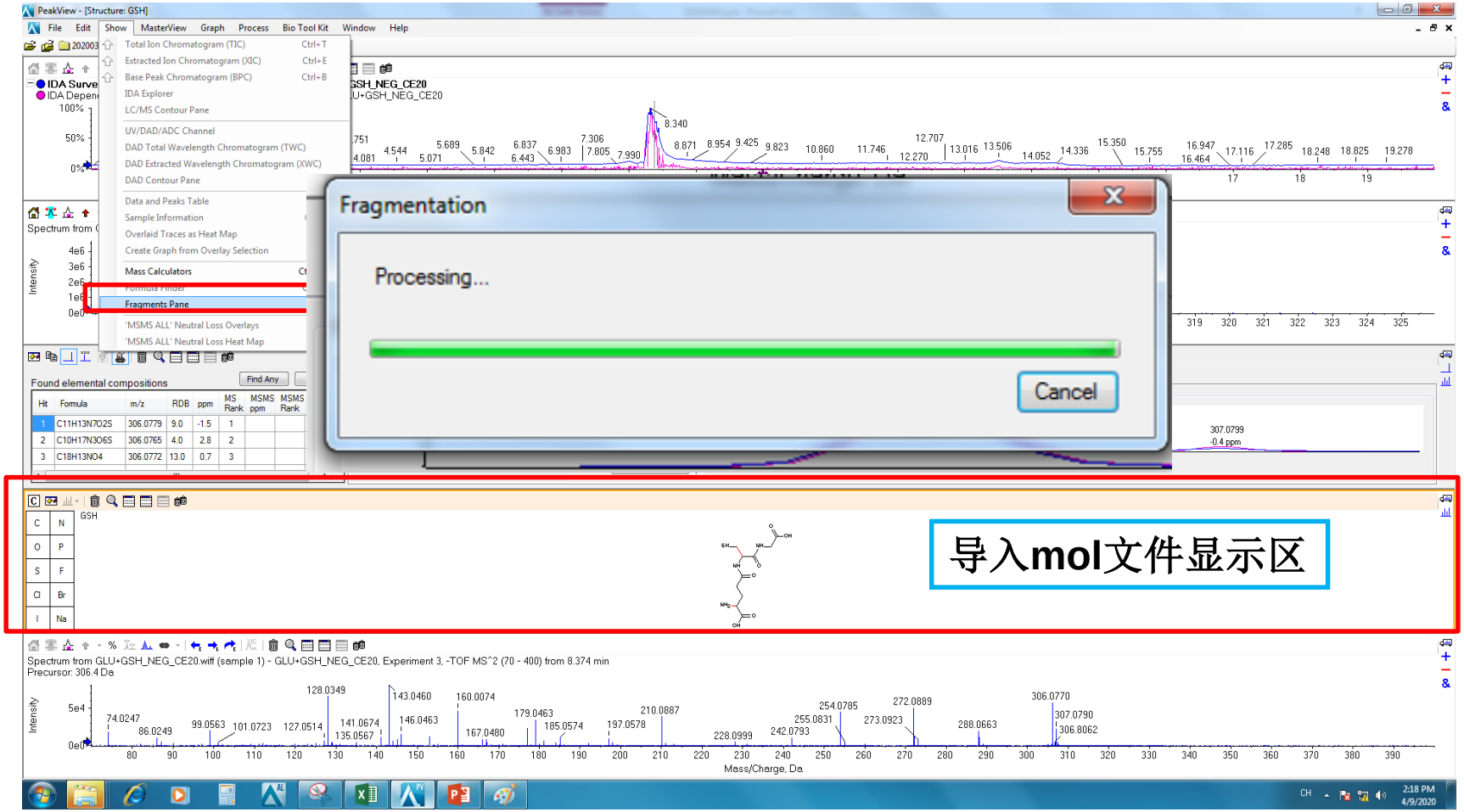
1、按住方框内图标，拖到二级质谱图上
2、点击find
3、点击MSMS Details

绿色代表吻合的碎片

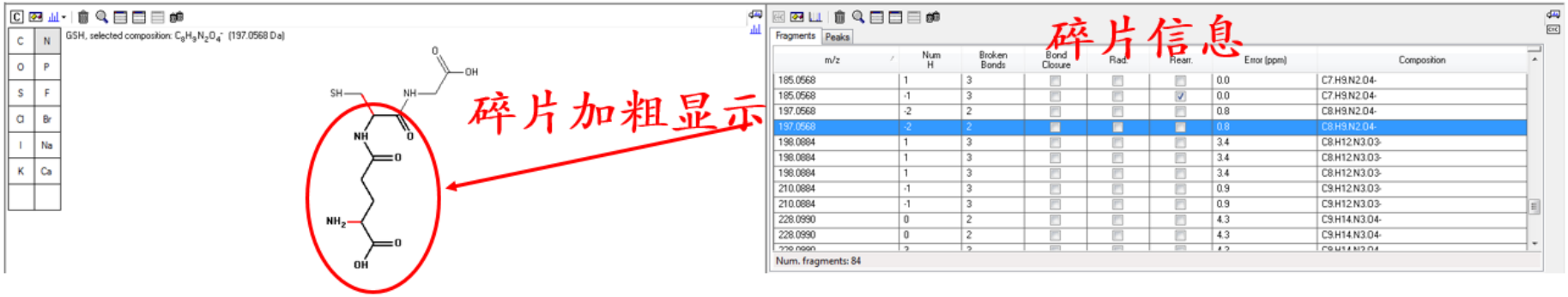


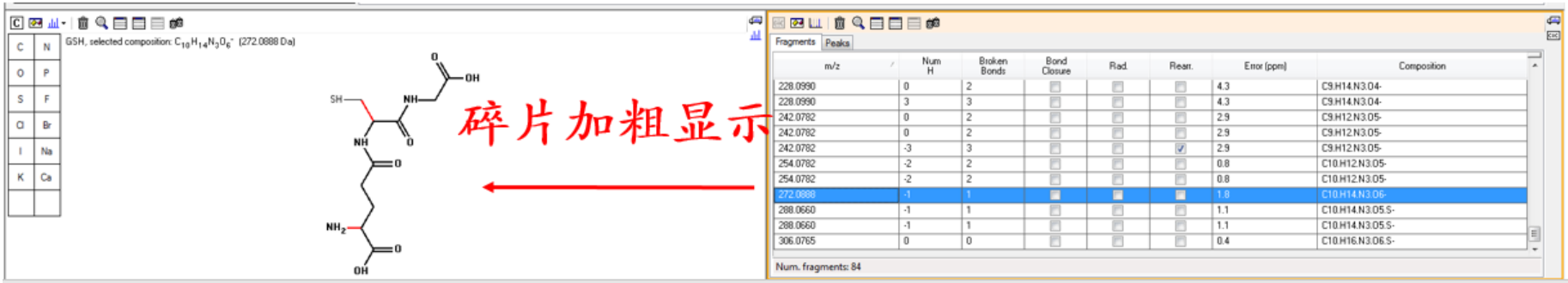
Hit	Formula	m/z	RDB	ppm	MS Rank	MSMS ppm	MSMS Rank	Found
1	C10H17N3O6S	306.0765	4.0	1.9	2	2.2...	1	NA/NA
2	C11H13N7O2S	306.0779	9.0	-2.5	1	20....	2	NA/NA
3	C18H13NO4	306.0772	13.0	-0.3	4	15....	3	NA/NA
4	C14H9N7O2	306.0745	14.0	8.5	3	17....	4	NA/NA
5	C19H9N5	306.0785	18.0	-4.6	5	38....	5	NA/NA


PeakView - [Formula Finder]
File Edit Show MasterView Graph Process Bio Tool Kit Window Help
Open Sample... Ctrl+O
Open Multiple Samples... Ctrl+Shift+O
Open Heat Map TICs from Wiff...
Find Wiff Samples Ctrl+L
Open T2D Data
Open Text Data
Open Mol File...
Export
Print
Exit Alt+F4
Time, min
Spectrum from GLU+GSH_NEG_CE20.wiff (sample 1) - GLU+GSH_NEG_CE20, Experiment 1, -TOF MS (70 - 650) from 8.372 min
Intensity
Mass/Charge, Da
Found elemental compositions
Find Any
Find
Hit Formula m/z RDB ppm MS Rank MSMS ppm MSMS Rank Found
1 C11H13N7O2S 306.0779 9.0 -1.5 1 NA/NA
2 C10H17N3O6S 306.0765 4.0 2.8 2 NA/NA
3 C18H13NO4 306.0772 13.0 0.7 3 NA/NA
4 C7H13N7O7 306.0804 5.0 -9.7 4 (2) NA/NA
5 C14H9N7O2 306.0745 14.0 9.5 4 (2) NA/NA
6 C19H9N5 306.0785 18.0 -3.7 6 NA/NA
MS Details
MSMS Details
Compound Details
Isotope cluster details
Charge
Elements from
Elements to
C20H30N10O10S2
Mass tolerance (ppm)
10
Intensity tolerance (%)
30
#C/#heteroatoms greater than
0
MS result summary for C11H12N7O2S, [M-H]-
306.0774
-1.5 ppm
Ion type:
[M-H]-
4 additional ions...
Spectrum from GLU+GSH_NEG_CE20.wiff (sample 1) - GLU+GSH_NEG_CE20, Experiment 3, -TOF MS^2 (70 - 400) from 8.374 min
Precursor: 306.4 Da

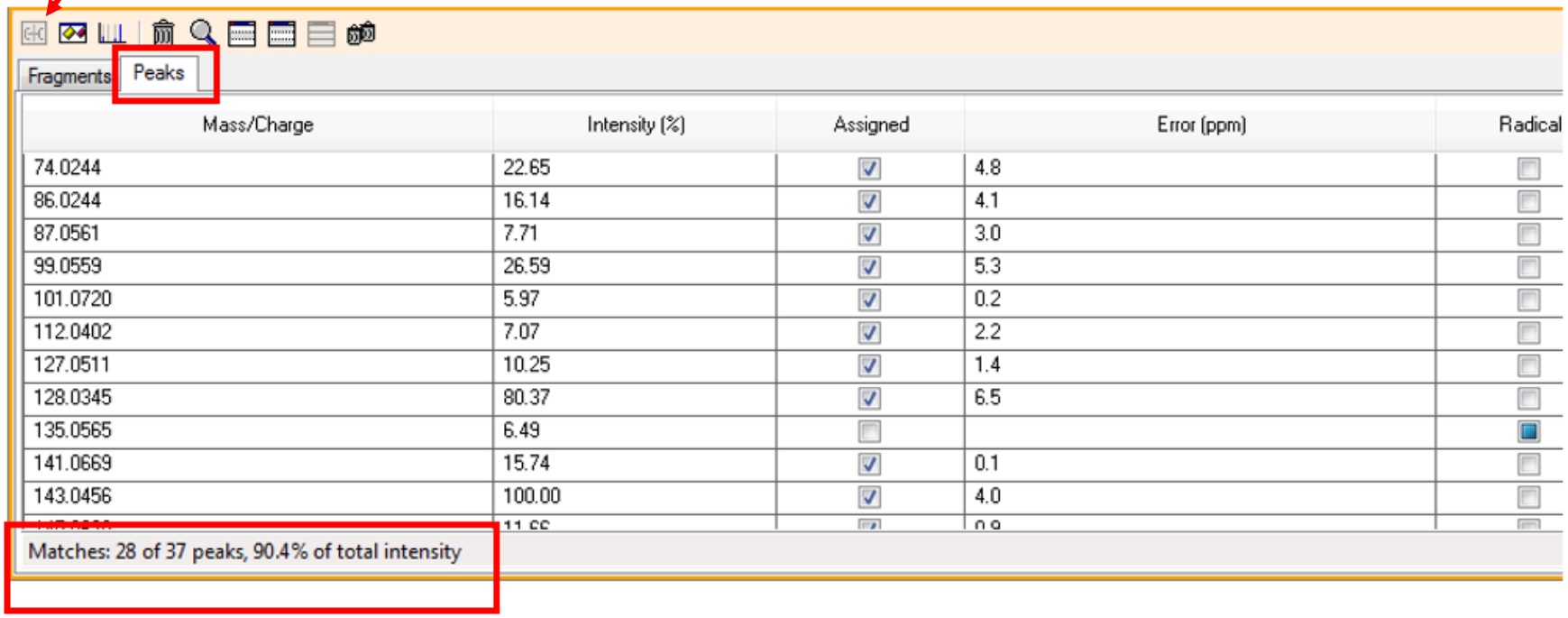

PeakView - [Structure: GSH]
File Edit Show MasterView Graph Process Bio Tool Kit Window Help
Total Ion Chromatogram (TIC) Ctrl+T
Extracted Ion Chromatogram (XIC) Ctrl+E
Base Peak Chromatogram (BPC) Ctrl+B
IDA Explorer
LC/MS Contour Pane
UV/DAD/ADC Channel
DAD Total Wavelength Chromatogram (TWC)
DAD Extracted Wavelength Chromatogram (XWC)
DAD Contour Pane
Data and Peaks Table
Sample Information
Overlaid Traces as Heat Map
Create Graph from Overlay Selection
Mass Calculators
Fragments Pane
'MSMS ALL' Neutral Loss Overlays
'MSMS ALL' Neutral Loss Heat Map
Fragmentation
Processing...
Cancel
Found elemental compositions
Find Any
Hit Formula m/z RDB ppm MS Rank MSMS ppm MSMS Rank
1 C11H13N7O2S 306.0779 9.0 -1.5 1
2 C10H17N3O6S 306.0765 4.0 2.8 2
3 C18H13NO4 306.0772 13.0 0.7 3
GSH
导入mol文件显示区
Spectrum from GLU+GSH_NEG_CE20.wiff (sample 1) - GLU+GSH_NEG_CE20, Experiment 3, -TOF MS^2 (70 - 400) from 8.374 min
Precursor: 306.4 Da
Intensity
Mass/Charge, Da

实测二级与导入化合物理论二级的匹配



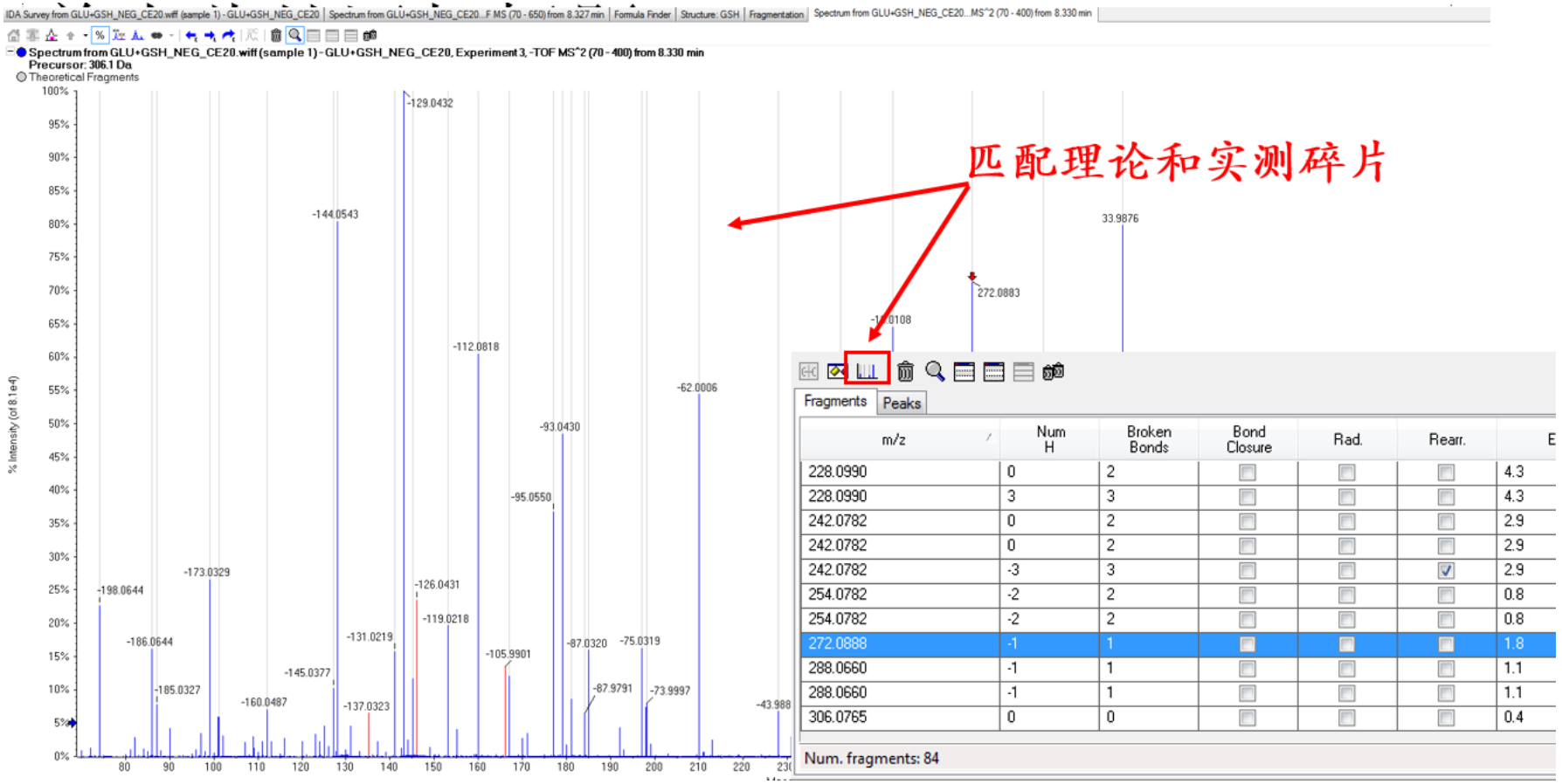


点击进行峰匹配

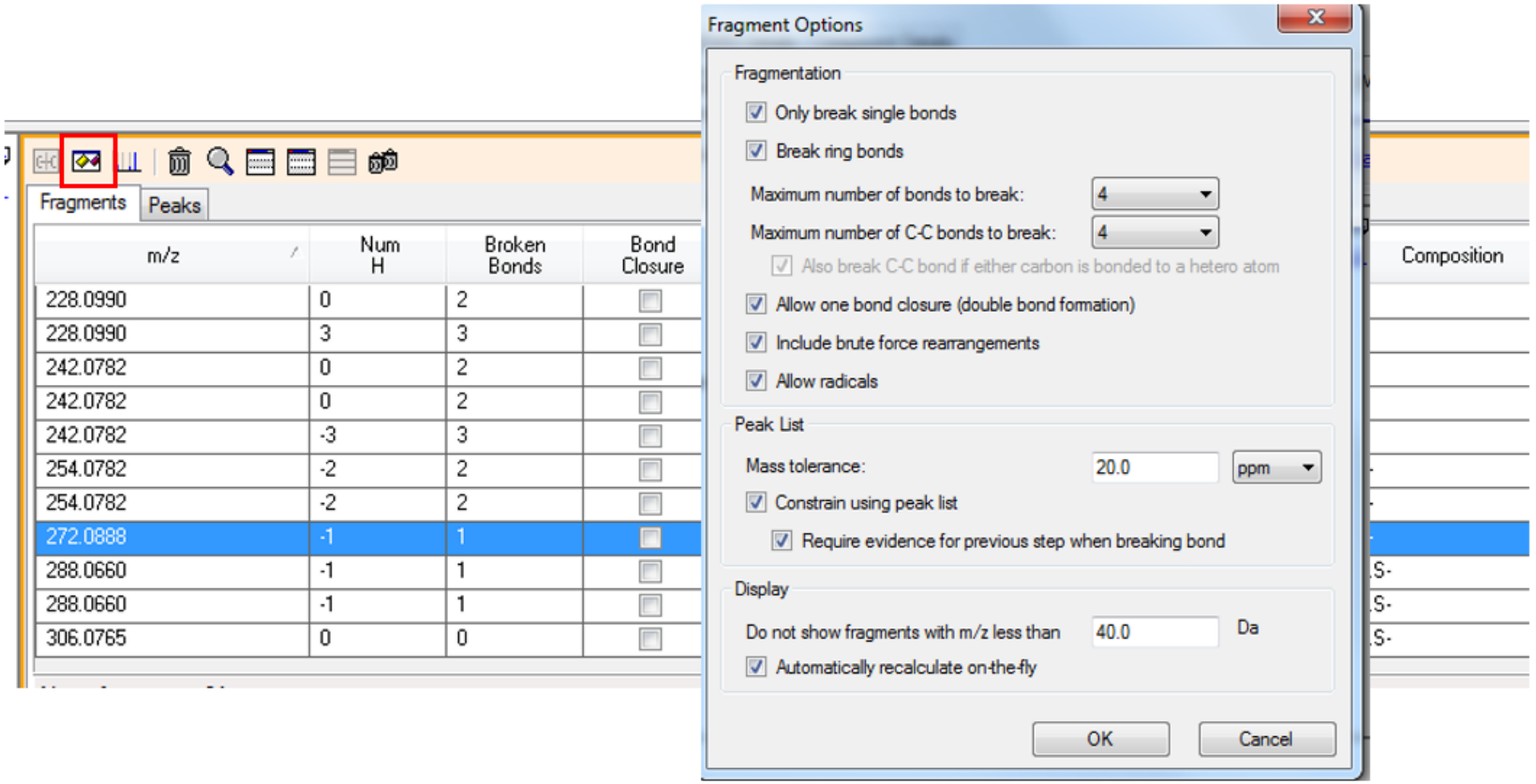


匹配分值查看

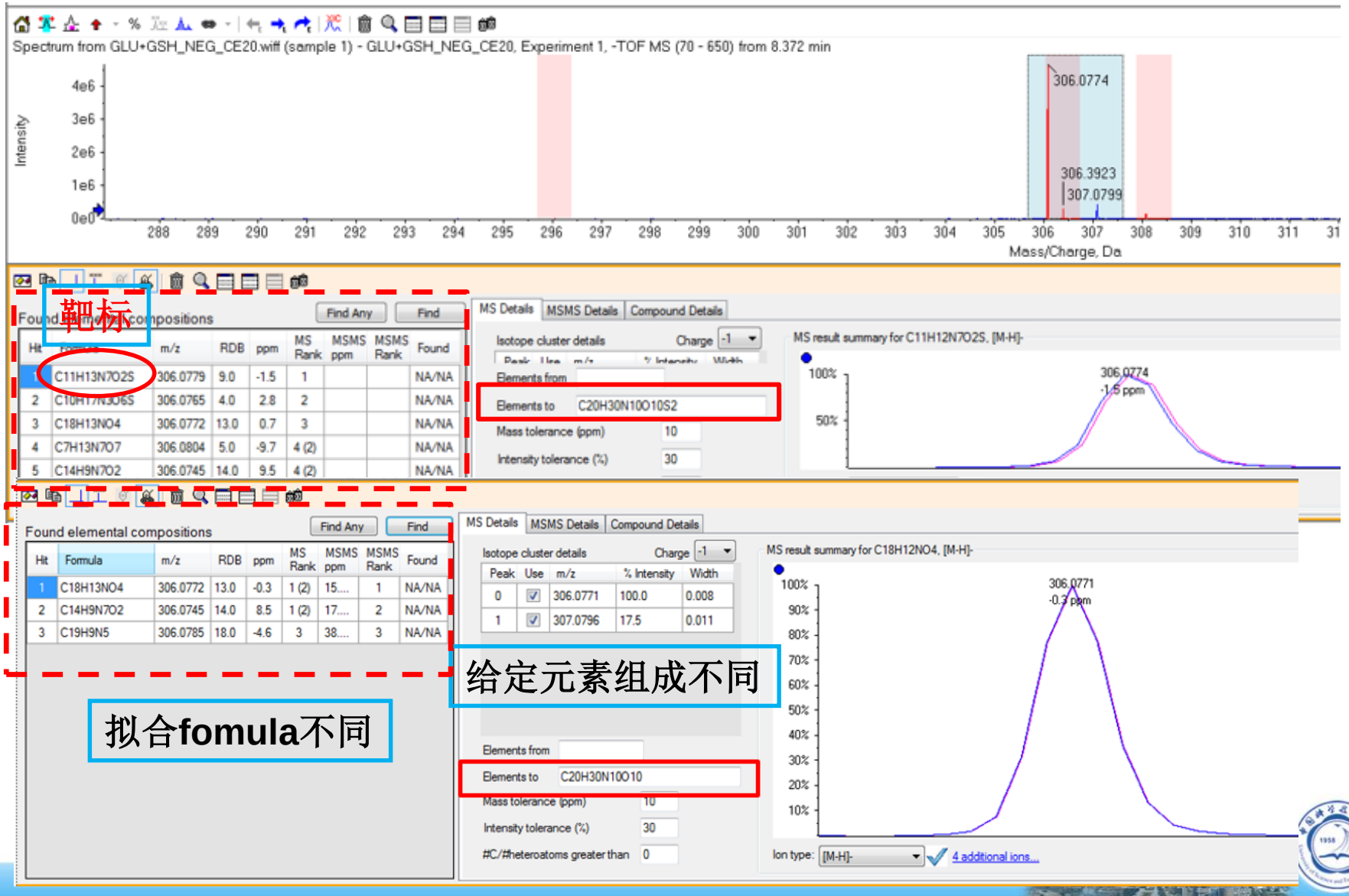
实测二级与导入化合物理论二级的匹配



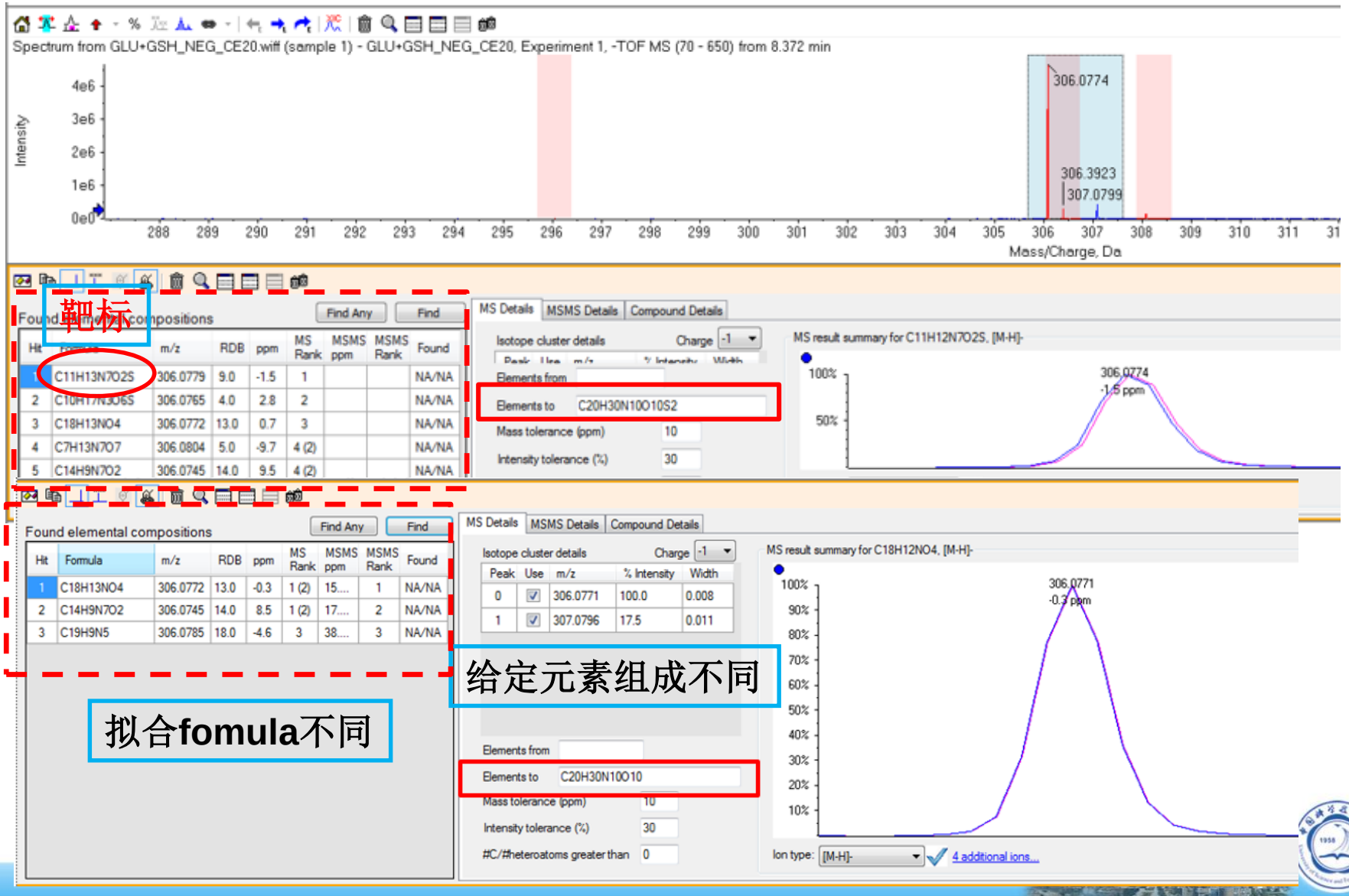
化合物断裂规律参数


Fragments
Peaks
m/z
Num H
Broken Bonds
Bond Closure
228.0990 0 2
228.0990 3 3
242.0782 0 2
242.0782 0 2
242.0782 -3 3
254.0782 -2 2
254.0782 -2 2
272.0888 -1 1
288.0660 -1 1
288.0660 -1 1
306.0765 0 0
Composition
Fragment Options
Fragmentation
Only break single bonds
Break ring bonds
Maximum number of bonds to break: 4
Maximum number of C-C bonds to break: 4
Also break C-C bond if either carbon is bonded to a hetero atom
Allow one bond closure (double bond formation)
Include brute force rearrangements
Allow radicals
Peak List
Mass tolerance: 20.0 ppm
Constrain using peak list
Require evidence for previous step when breaking bond
Display
Do not show fragments with m/z less than 40.0 Da
Automatically recalculate on-the-fly
OK
Cancel

注意事项


Spectrum from GLU+GSH_NEG_CE20.wiff (sample 1) - GLU+GSH_NEG_CE20, Experiment 1, -TOF MS (70 - 650) from 8.372 min
Intensity
Mass/Charge, Da
306.0774
306.3923
307.0799
靶标
Found elemental compositions
Find Any
Find
Hit
Formula
m/z
RDB
ppm
MS Rank
MSMS ppm
MSMS Rank
Found
1 C11H13N7O2S 306.0779 9.0 -1.5 1 NA/NA
2 C10H17N3O6S 306.0765 4.0 2.8 2 NA/NA
3 C18H13NO4 306.0772 13.0 0.7 3 NA/NA
4 C7H13N7O7 306.0804 5.0 -9.7 4 (2) NA/NA
5 C14H9N7O2 306.0745 14.0 9.5 4 (2) NA/NA
MS Details
MSMS Details
Compound Details
Isotope cluster details
Charge
Elements from
Elements to C20H30N10O10S2
Mass tolerance (ppm) 10
Intensity tolerance (%) 30
MS result summary for C11H12N7O2S, [M-H]-
306.0774
-1.5 ppm
1 C18H13NO4 306.0772 13.0 -0.3 1 (2) 15.... 1 NA/NA
2 C14H9N7O2 306.0745 14.0 8.5 1 (2) 17.... 2 NA/NA
3 C19H9N5 306.0785 18.0 -4.6 3 38.... 3 NA/NA
Peak Use m/z % Intensity Width
0 306.0771 100.0 0.008
1 307.0796 17.5 0.011
Elements to C20H30N10O10
#C/#heteroatoms greater than 0
MS result summary for C18H12NO4, [M-H]-
306.0771
-0.3 ppm
Ion type: [M-H]-
4 additional ions...
拟合fomula不同
给定元素组成不同

注意事项


Spectrum from GLU+GSH_NEG_CE20.wiff (sample 1) - GLU+GSH_NEG_CE20, Experiment 1, -TOF MS (70 - 650) from 8.372 min
Intensity
Mass/Charge, Da
306.0774
306.3923
307.0799
靶标
Found elemental compositions
Find Any
Find
Hit
Formula
m/z
RDB
ppm
MS Rank
MSMS ppm
MSMS Rank
Found
1 C11H13N7O2S 306.0779 9.0 -1.5 1 NA/NA
2 C10H17N3O6S 306.0765 4.0 2.8 2 NA/NA
3 C18H13NO4 306.0772 13.0 0.7 3 NA/NA
4 C7H13N7O7 306.0804 5.0 -9.7 4 (2) NA/NA
5 C14H9N7O2 306.0745 14.0 9.5 4 (2) NA/NA
MS Details
MSMS Details
Compound Details
Isotope cluster details
Charge
Elements from
Elements to C20H30N10O10S2
Mass tolerance (ppm) 10
Intensity tolerance (%) 30
MS result summary for C11H12N7O2S, [M-H]-
306.0774
-1.5 ppm
1 C18H13NO4 306.0772 13.0 -0.3 1 (2) 15.... 1 NA/NA
2 C14H9N7O2 306.0745 14.0 8.5 1 (2) 17.... 2 NA/NA
3 C19H9N5 306.0785 18.0 -4.6 3 38.... 3 NA/NA
Peak Use m/z % Intensity Width
0 306.0771 100.0 0.008
1 307.0796 17.5 0.011
Elements to C20H30N10O10
#C/#heteroatoms greater than 0
MS result summary for C18H12NO4, [M-H]-
306.0771
-0.3 ppm
Ion type: [M-H]-
4 additional ions...
拟合fomula不同
给定元素组成不同