



PeakView软件手动鉴定化合物结构式

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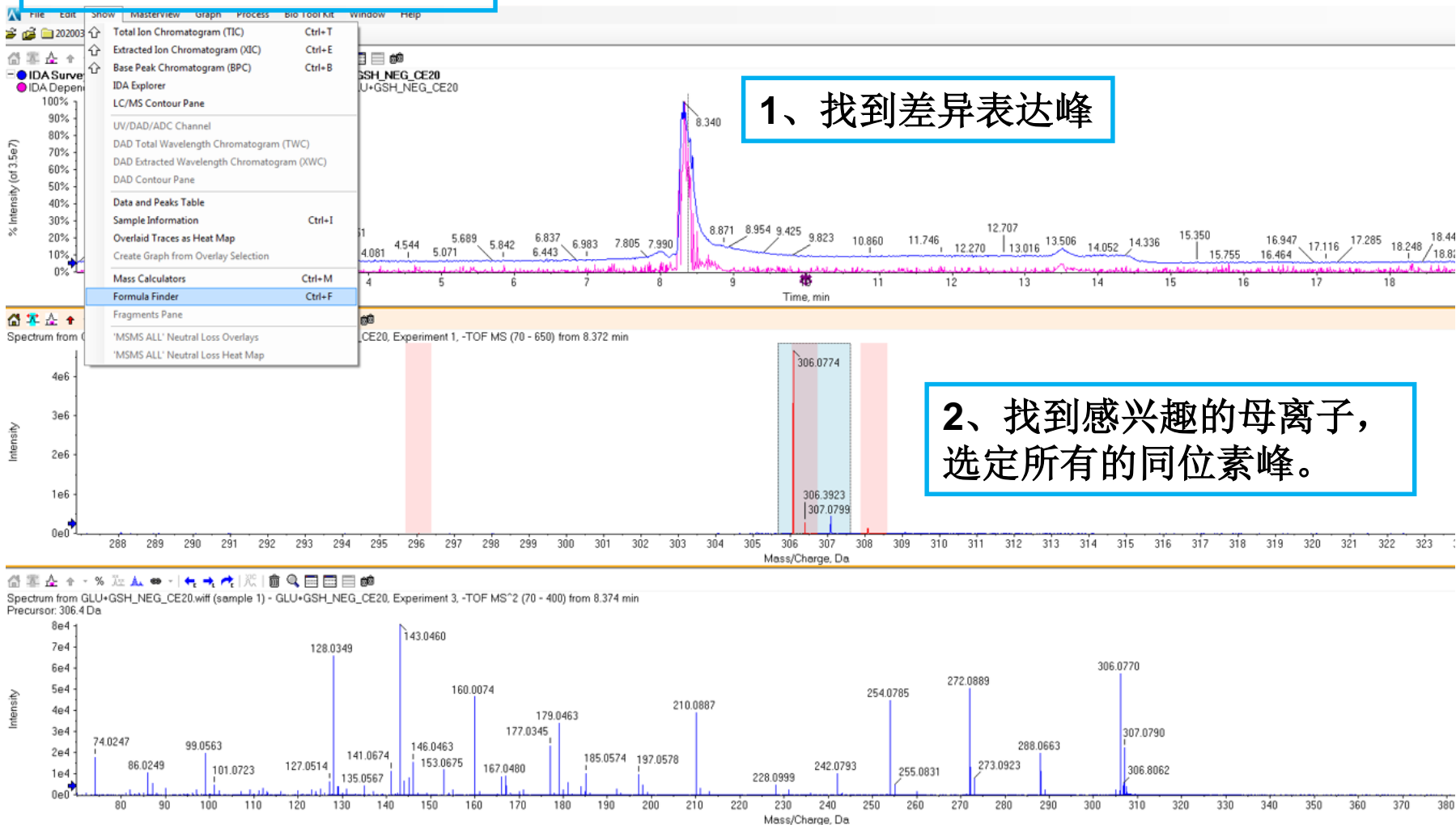
<http://biotech.ustc.edu.cn>

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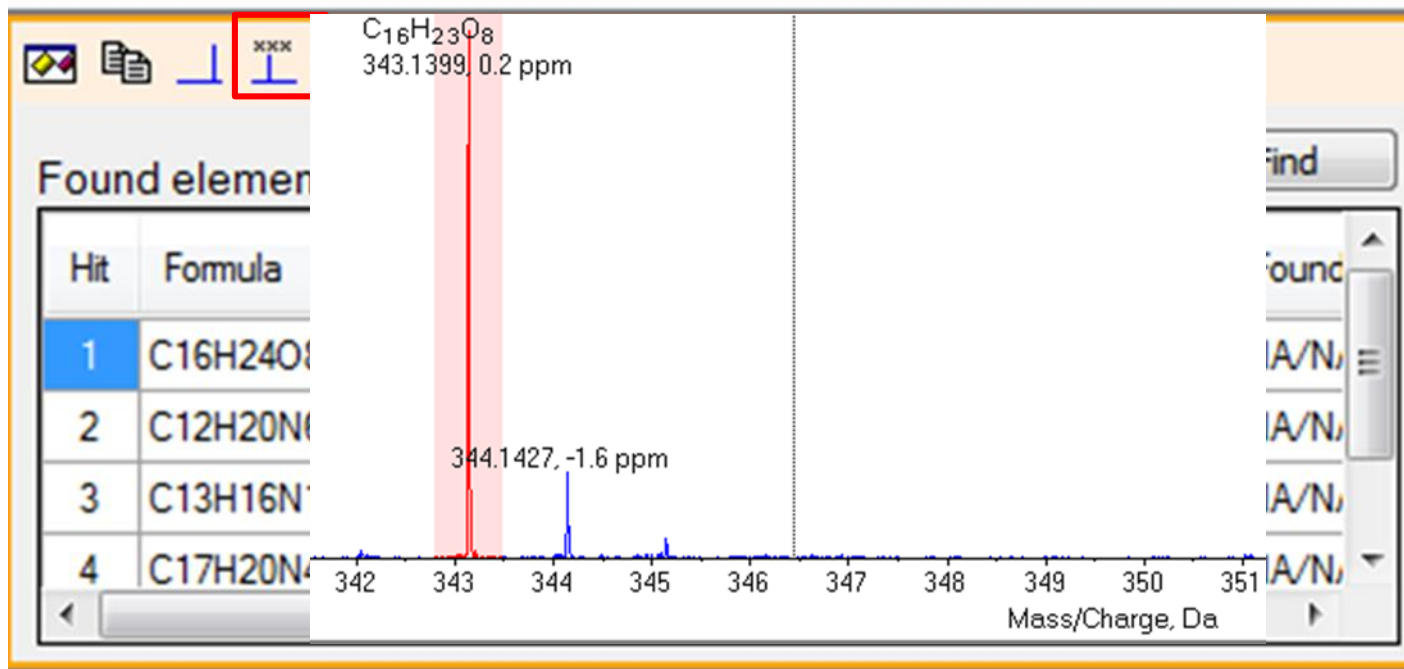


一、打开一个数据

3、Show-formula finder



二、拟合结果



点击红色图标，可在一级质谱上标记选中的formula及error

注意：我们一般会用Masterview去提差异峰，据已有经验判断，masterview即便能拟合出分子式，分子式的可信度也是很差的，因此推荐大家找到感兴趣的差异峰后，用Peakview拟合出来的分子式。



可能碰到的问题:拟合无结果

Found elemental compositions

| Hit | Formula | m/z | RDB | ppm | MS Rank | MSMS ppm | MSMS Rank | Found |
|-----|---------|-----|-----|-----|---------|----------|-----------|-------|
|-----|---------|-----|-----|-----|---------|----------|-----------|-------|

MS Details MSMS Details Compound Details

Isotope cluster details Charge **-1**

| Peak | File | m/z | % Intensity | Width |
|------|------|-----|-------------|-------|
|------|------|-----|-------------|-------|

Elements from

Elements to

Mass tolerance (ppm)

Intensity tolerance (%)

#C/#heteroatoms greater than

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

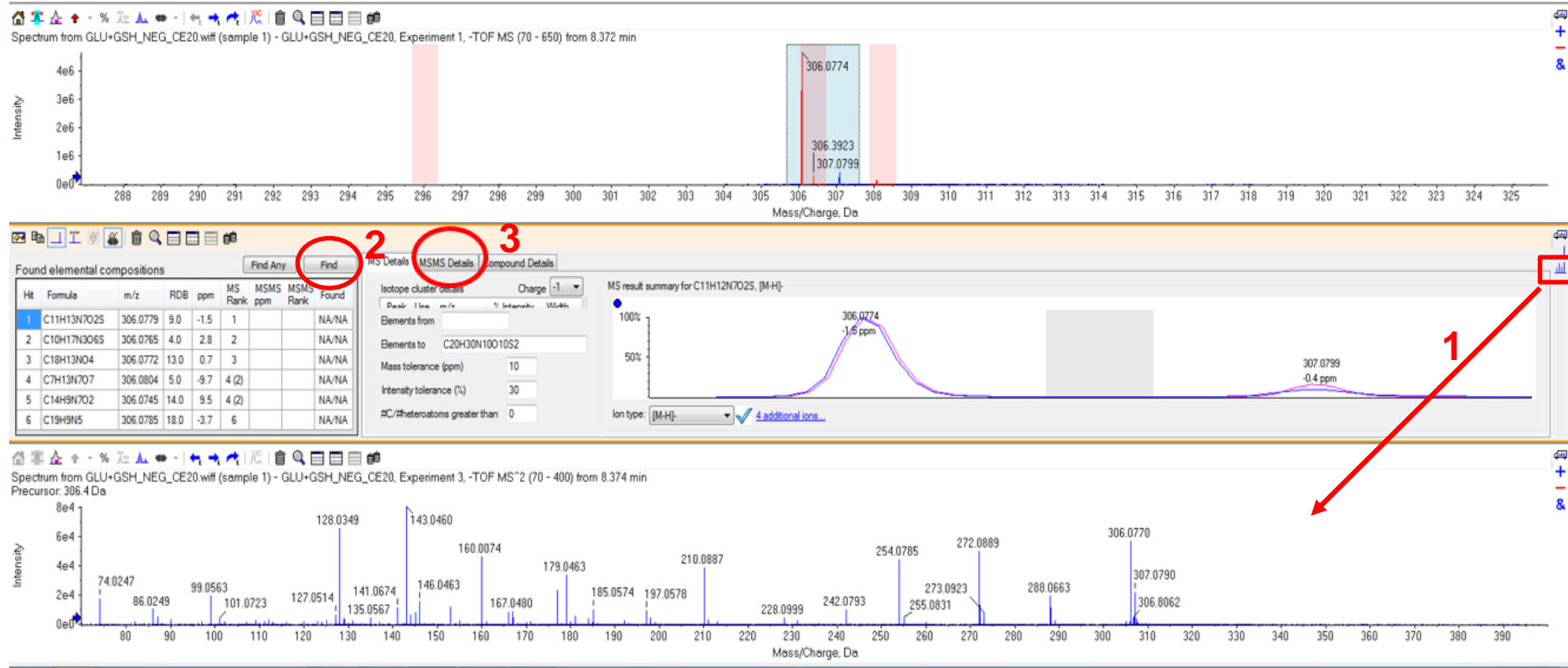
Ion type: [4 additional ions...](#)

需要告诉离子加和形式

如果已经告知了离子加和形式在限定的分子组成和允许误差范围内依然拟合不出来,可适当放宽限定条件。

三、匹配拟合分子式的理论和实测二级

1、二级谱图的碎片的精确质量数匹配



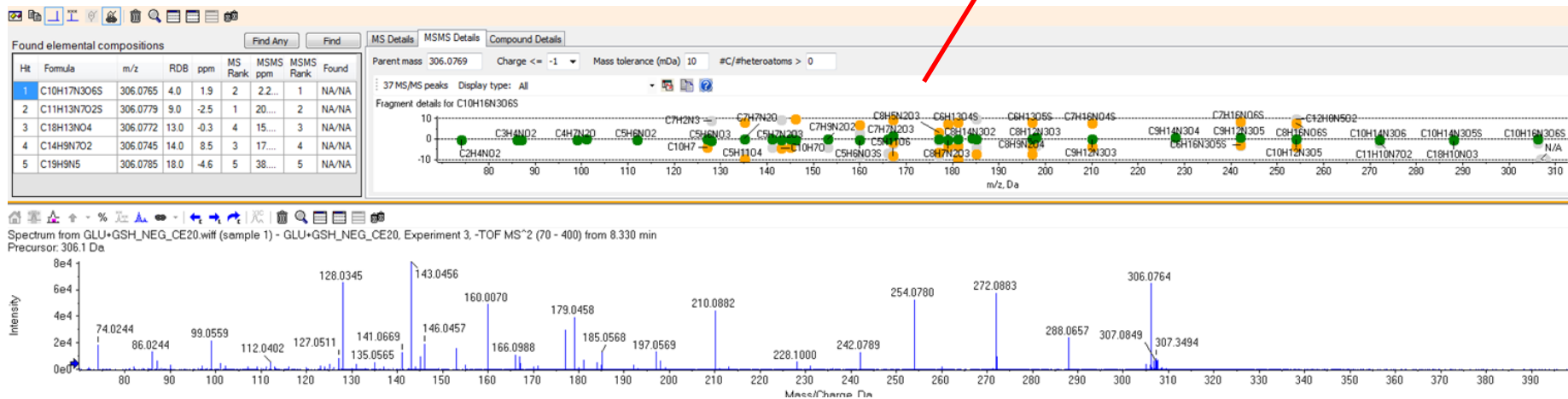
操作步骤:

- 1) 按住方框内谱图图标, 拖到二级质谱图上
- 2) 点击find
- 3) 点击MSMS Details



二级碎片精确质量数匹配结果显示

绿色代表吻合的碎片



注意：该步的匹配，只是在右侧给定候选的化合物分子中选定的那个分子组成范围内，对仪器实测的二级谱图碎片的精确质量数做匹配，不含有拟定化合物的分子结构信息。绿色代表拟合出来的碎片分子量和实测的误差在允许范围内，黄色代表偏差较大，灰色代表未拟合出来。



2、二级谱图的碎片的结构信息匹配（已有预测结构式的前提下可执行该步骤）

导入目标物mol文件

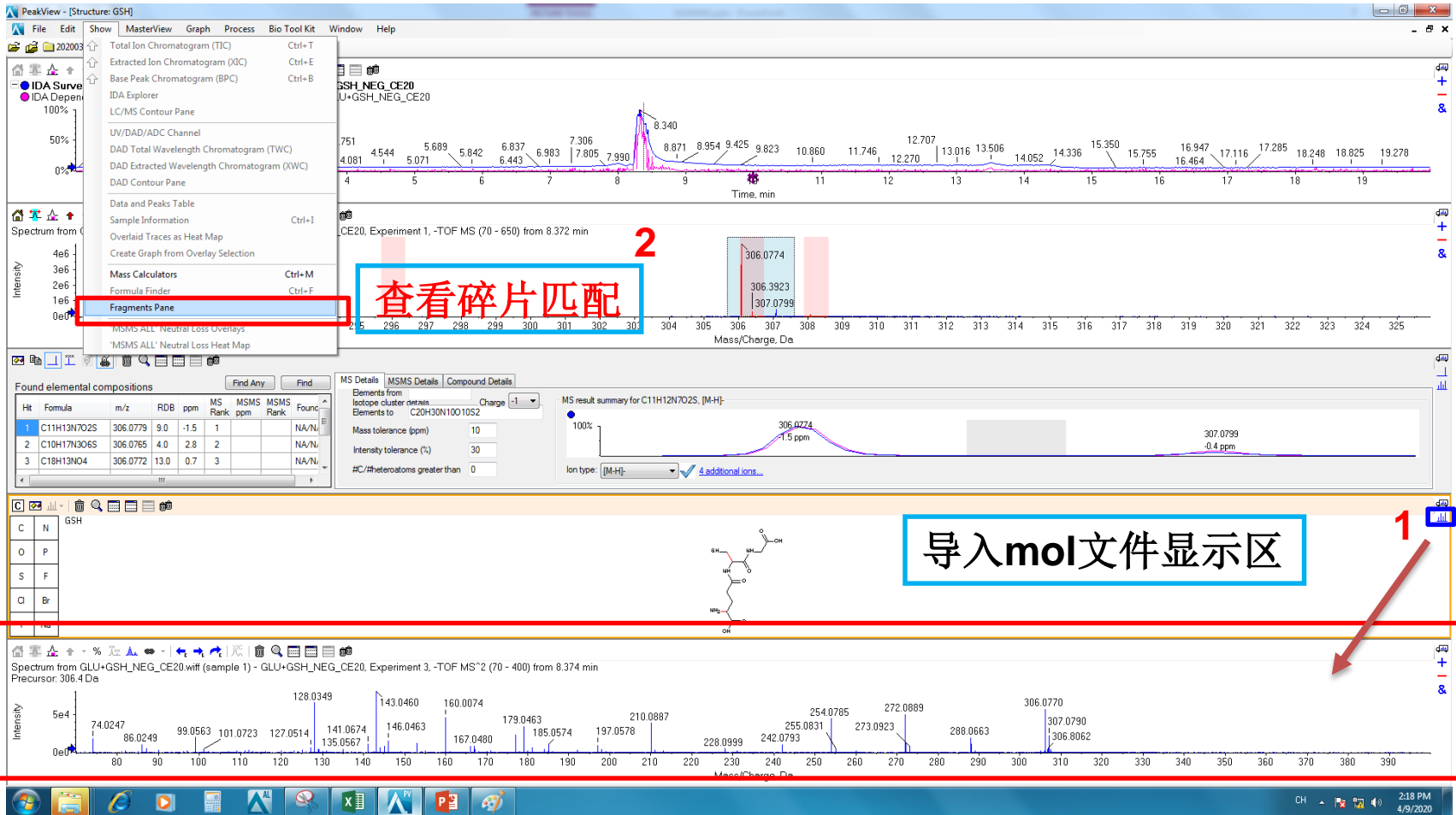
Found elemental compositions

| Hit | Formula | m/z | RDB | ppm | MS Rank | MSMS Rank | 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 result summary for C11H12N7O2S, [M-H]:

Isotope cluster details: Charge -1, Elements from C20H30N10O10S2, Mass tolerance (ppm) 10, Intensity tolerance (%) 30, #C/#heteroatoms greater than 0.

Peak list (m/z): 74.0247, 86.0249, 99.0563, 101.0723, 127.0514, 135.0567, 141.0674, 143.0460, 146.0463, 160.0074, 167.0480, 179.0463, 185.0574, 197.0578, 210.0887, 228.0999, 242.0793, 254.0785, 255.0831, 273.0923, 272.0889, 288.0663, 306.0770, 307.0790, 306.8062.



- 1) 导入摩尔文件结构式的右侧有谱图标志，左键按住拖拽到实测谱图上。
- 2) show-fragmentation pane



匹配结果查看—评分查看

点击进行峰匹配

| Mass/Charge | Intensity (%) | Assigned | Error (ppm) | Radical |
|-------------|---------------|-------------------------------------|-------------|-------------------------------------|
| 74.0244 | 22.65 | <input checked="" type="checkbox"/> | 4.8 | <input type="checkbox"/> |
| 86.0244 | 16.14 | <input checked="" type="checkbox"/> | 4.1 | <input type="checkbox"/> |
| 87.0561 | 7.71 | <input checked="" type="checkbox"/> | 3.0 | <input type="checkbox"/> |
| 99.0559 | 26.59 | <input checked="" type="checkbox"/> | 5.3 | <input type="checkbox"/> |
| 101.0720 | 5.97 | <input checked="" type="checkbox"/> | 0.2 | <input type="checkbox"/> |
| 112.0402 | 7.07 | <input checked="" type="checkbox"/> | 2.2 | <input type="checkbox"/> |
| 127.0511 | 10.25 | <input checked="" type="checkbox"/> | 1.4 | <input type="checkbox"/> |
| 128.0345 | 80.37 | <input checked="" type="checkbox"/> | 6.5 | <input type="checkbox"/> |
| 135.0565 | 6.49 | <input type="checkbox"/> | | <input checked="" type="checkbox"/> |
| 141.0669 | 15.74 | <input checked="" type="checkbox"/> | 0.1 | <input type="checkbox"/> |
| 143.0456 | 100.00 | <input checked="" type="checkbox"/> | 4.0 | <input type="checkbox"/> |
| 147.0330 | 11.66 | <input checked="" type="checkbox"/> | 0.0 | <input type="checkbox"/> |

Matches: 28 of 37 peaks, 90.4% of total intensity

匹配分值查看

注意：该步的匹配，是用软件计算的理论二级碎片和实际测到的二级谱图进行匹配，改变化合物断裂规律设置，可改变理论二级碎片的组成和丰度。



可调整参数--化合物断裂规律参数

The screenshot displays a software interface for mass spectrometry data analysis. On the left, a table titled 'Fragments' shows the following data:

| m/z | Num H | Broken Bonds | Bond Closure |
|----------|-------|--------------|--------------------------|
| 228.0990 | 0 | 2 | <input type="checkbox"/> |
| 228.0990 | 3 | 3 | <input type="checkbox"/> |
| 242.0782 | 0 | 2 | <input type="checkbox"/> |
| 242.0782 | 0 | 2 | <input type="checkbox"/> |
| 242.0782 | -3 | 3 | <input type="checkbox"/> |
| 254.0782 | -2 | 2 | <input type="checkbox"/> |
| 254.0782 | -2 | 2 | <input type="checkbox"/> |
| 272.0888 | -1 | 1 | <input type="checkbox"/> |
| 288.0660 | -1 | 1 | <input type="checkbox"/> |
| 288.0660 | -1 | 1 | <input type="checkbox"/> |
| 306.0765 | 0 | 0 | <input type="checkbox"/> |

The 'Fragment Options' dialog box is open, showing the following settings:

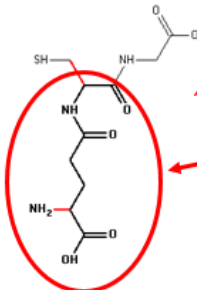
- Fragmentation**
 - Only break single bonds
 - Break ring bonds
 - Maximum number of bonds to break: 4
 - Maximum number of C-C bonds to break: 4
 - Also break C-C bond if either carbon is bonded to a hetero atom
 - Allow one bond closure (double bond formation)
 - Include brute force rearrangements
 - 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

Buttons for 'OK' and 'Cancel' are visible at the bottom of the dialog box.

可通过调整这些参数，改变化合物断裂规律，从而改变理论二级碎片。

匹配结果查看--碎片断裂情况查看

GSH, selected composition: $C_3H_5N_2O_4^-$ (197.0568 Da)



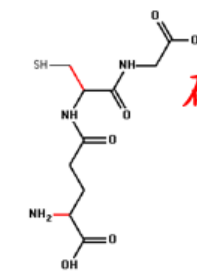
碎片加粗显示

碎片信息

| m/z | Num H | Broken Bonds | Bond Closure | Rad | Rearr. | Error (ppm) | Composition |
|----------|-------|--------------|--------------|-----|--------|-------------|-------------|
| 185.0568 | 1 | 3 | | | | 0.0 | C7H9N2O4- |
| 185.0568 | -1 | 3 | | | | 0.0 | C7H9N2O4- |
| 197.0568 | -2 | 2 | | | | 0.8 | C8H9N2O4- |
| 197.0568 | -2 | 2 | | | | 0.8 | C8H9N2O4- |
| 198.0884 | 1 | 3 | | | | 3.4 | C8H12N3O3- |
| 198.0884 | 1 | 3 | | | | 3.4 | C8H12N3O3- |
| 198.0884 | 1 | 3 | | | | 3.4 | C8H12N3O3- |
| 210.0884 | -1 | 3 | | | | 0.9 | C9H12N3O3- |
| 210.0884 | -1 | 3 | | | | 0.9 | C9H12N3O3- |
| 228.0990 | 0 | 2 | | | | 4.3 | C9H14N3O4- |
| 228.0990 | 0 | 2 | | | | 4.3 | C9H14N3O4- |
| 228.0990 | 0 | 2 | | | | 4.3 | C9H14N3O4- |

Num. fragments: 84

GSH, selected composition: $C_{10}H_{14}N_3O_6^-$ (272.0888 Da)



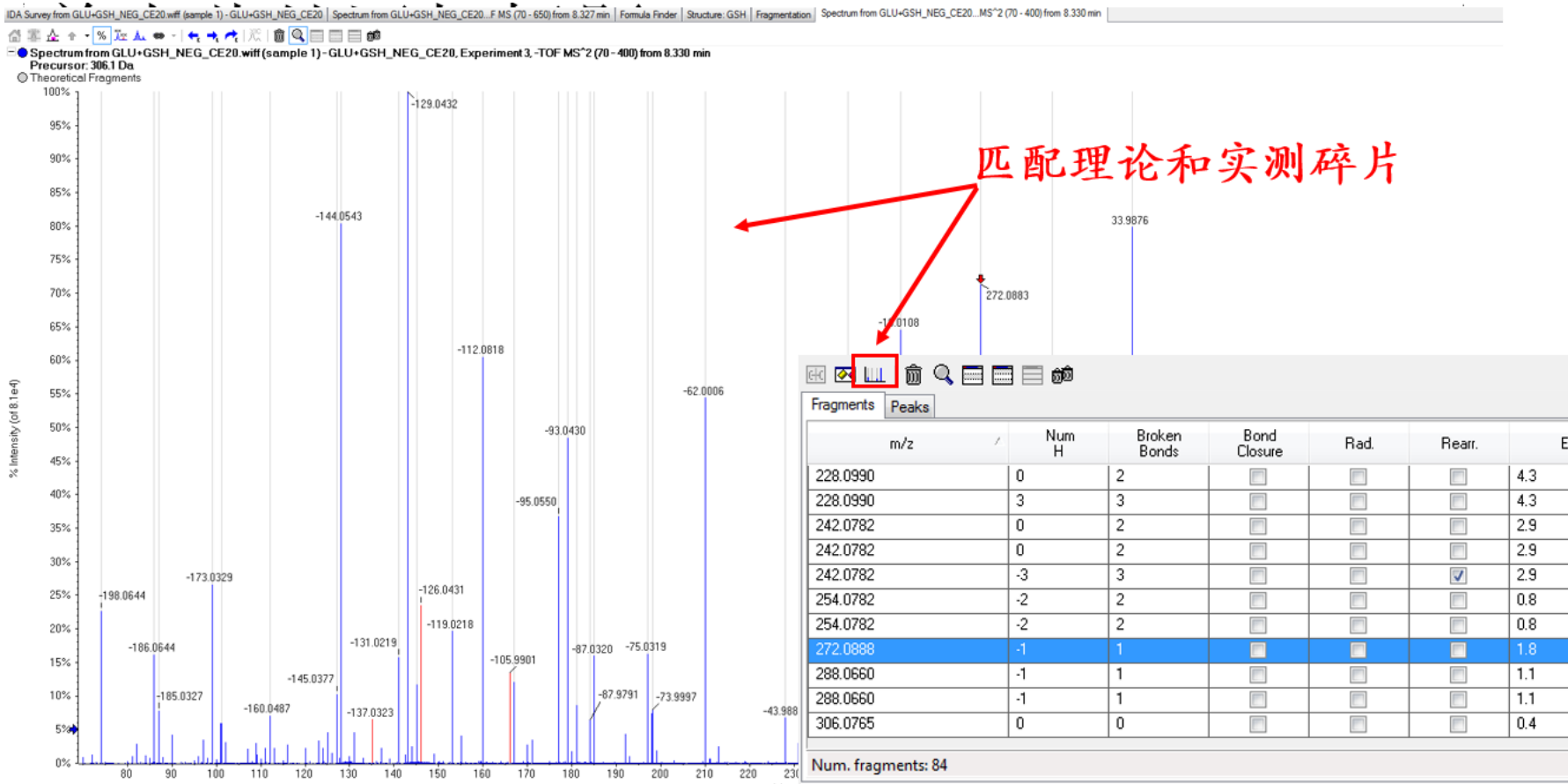
碎片加粗显示

碎片信息

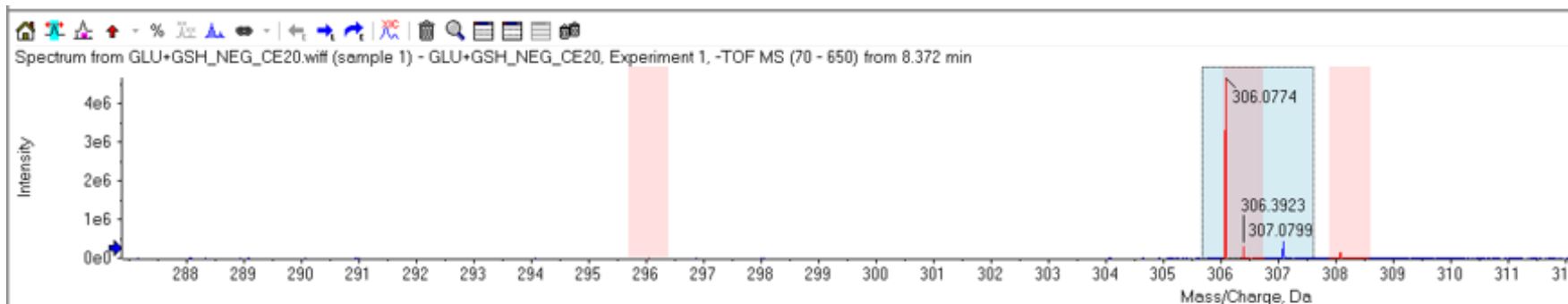
| m/z | Num H | Broken Bonds | Bond Closure | Rad | Rearr. | Error (ppm) | Composition |
|----------|-------|--------------|--------------|-----|--------|-------------|--------------|
| 228.0990 | 0 | 2 | | | | 4.3 | C9H14N3O4- |
| 228.0990 | 3 | 3 | | | | 4.3 | C9H14N3O4- |
| 242.0782 | 0 | 2 | | | | 2.9 | C9H12N3O5- |
| 242.0782 | 0 | 2 | | | | 2.9 | C9H12N3O5- |
| 242.0782 | -3 | 3 | | | | 2.9 | C9H12N3O5- |
| 254.0782 | -2 | 2 | | | | 0.8 | C10H12N3O5- |
| 254.0782 | -2 | 2 | | | | 0.8 | C10H12N3O5- |
| 272.0888 | -1 | 1 | | | | 1.9 | C10H14N3O6- |
| 288.0660 | -1 | 1 | | | | 1.1 | C10H14N3O5S- |
| 288.0660 | -1 | 1 | | | | 1.1 | C10H14N3O5S- |
| 306.0755 | 0 | 0 | | | | 0.4 | C10H16N3O6S- |

Num. fragments: 84

匹配结果查看--谱图匹配信息查看



注意事项



Found elemental compositions

| 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

Isotope cluster details Charge: -1

Elements to: C20H30N10O10S2

Mass tolerance (ppm): 10

Intensity tolerance (%): 30

MS result summary for C11H13N7O2S, [M-H]⁻

Found elemental compositions

| Hit | Formula | m/z | RDB | ppm | MS Rank | MSMS ppm | MSMS Rank | Found |
|-----|-----------|----------|------|------|---------|----------|-----------|-------|
| 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 |

MS Details

Isotope cluster details Charge: -1

| Peak | Use | m/z | % Intensity | Width |
|------|-------------------------------------|----------|-------------|-------|
| 0 | <input checked="" type="checkbox"/> | 306.0771 | 100.0 | 0.008 |
| 1 | <input checked="" type="checkbox"/> | 307.0796 | 17.5 | 0.011 |

Elements to: C20H30N10O10

Mass tolerance (ppm): 10

Intensity tolerance (%): 30

#C/#heteroatoms greater than: 0

MS result summary for C18H12NO4, [M-H]⁻

靶标

拟合formula不同

给定元素组成不同





有些开源库，比如Pubchem，HMDB，Massbank等会收录化合物的实测二级谱图，虽然二级谱图会受到不同检测设备、碰撞能量的影响，但也具有一定的参考意义，也是二级匹配判定的一种方式。不管怎么说，定性的金标准是确定候选物后，用标准品在本地再次和样本进行验证。

数据分析物质确认是一个繁琐耗时的过程，祝大家都能找到自己感兴趣的靶标。

