Data File: F:\高分辨数据\Zouyong\sjf\S1.lcd

| Elmt | Val. | Min | Max  | Elmt | Val. | Min | Max  | Elmt | Val. | Min | Max  |
|------|------|-----|------|------|------|-----|------|------|------|-----|------|
| H    | 1    | 0   | 80   | O    | 2    | 0   | 20   | P    | 3    | 0   | 0    |
| 2H   | 1    | 0   | 0    | 18O  | 2    | 0   | 0    | S    | 2    | 0   | 0    |
| B    | 3    | 0   | 0    | F    | 1    | 0   | 0    | Cl   | 1    | 0   | 0    |
| C    | 4    | 0   | 60   | Na   | 1    | 0   | 0    | K    | 1    | 0   | 0    |
| N    | 3    | 0   | 0    | Si   | 4    | 0   | 0    | Mn   | 3    | 0   | 0    |

Error Margin (ppm): 100
DBE Range: -2.0 - 1000.0
Electron Ions: both
Apply N Rule: yes
Use MSn Info: no
Max Results: 500

Event#: 1 MS(E+) Ret. Time: 1.240 Scan#: 187

Measured region for 253.0494 m/z

C15 H8 O4 [M+H]+: Predicted region for 253.0495 m/z

| Rank | Score | Formula (M) | Ion  | Meas. m/z | Pred. m/z | Df. (mDa) | Df. (ppm) | Iso | DBE |
|------|-------|-------------|------|-----------|-----------|-----------|-----------|-----|-----|
| 1    | 35.19 | C15 H8 O4   | [M+H]+ | 253.0494  | 253.0495  | -0.1      | -0.40     | 35.19 | 12.0 |
Formula Predictor Report - SJF-1B.lcd

Data File: \Deep-20160624\data1\湘江\SJF-1B.lcd

| Elmt | Val. | Min. | Max. |
|------|------|------|------|
| H    | 1    | 6    | 8    |
| 2H   | 1    | 0    | 0    |
| 3H   | 1    | 0    | 0    |
| B    | 3    | 0    | 0    |
| C    | 4    | 0    | 0    |
| N    | 3    | 0    | 0    |

| Elmt | Val. | Min. | Max. |
|------|------|------|------|
| O    | 2    | 2    | 3    |
| F    | 1    | 0    | 0    |
| Si   | 4    | 0    | 0    |
| P    | 3    | 0    | 0    |
| S    | 2    | 0    | 0    |
| Cl   | 1    | 0    | 0    |

| Elmt | Val. | Min. | Max. |
|------|------|------|------|
| K    | 1    | 0    | 0    |
| Mn   | 3    | 0    | 0    |
| Fe   | 2    | 0    | 0    |
| Cu   | 2    | 0    | 0    |
| Se   | 2    | 0    | 0    |
| Br   | 1    | 0    | 0    |

| Elmt | Val. | Min. | Max. |
|------|------|------|------|
| Pd   | 2    | 0    | 0    |
| I    | 3    | 0    | 0    |
| Pt   | 2    | 0    | 0    |
| Au   | 1    | 0    | 0    |

Use Adduct: H

Error Margin (ppm): 100

HC Ratio: 0.0 - 100.0

Max Isotopes: all

MSn Iso RI (%): 75.00

MSn Logic Mode: AND

Max Results: 100

Event#: 1 MS(E+) Ret. Time: 1.120 -> 1.120 Scan#: 169 -> 169

Measured region for 237.0539 m/z

C15 H8 O3 [M+H]+ : Predicted region for 237.0546 m/z
Data File: 高分辨数据\Zouyong\sjf\S2.lcd

| Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Use Adduct |
|------|------|-----|-----|------|------|-----|-----|------|------|-----|-----|------|------|-----|-----|------------|
| H    | 1    | 0   | 80  | O    | 2    | 0   | 20  | P     | 3    | 0   | 0   | Zn    | 2    | 0   | 0   | H          |
| 2H   | 1    | 0   | 0   | 18O  | 2    | 0   | 0   | S     | 2    | 0   | 0   | Se    | 2    | 0   | 0   |            |
| B    | 3    | 0   | 0   | F    | 1    | 0   | 0   | Cl    | 1    | 0   | 0   | Br    | 1    | 0   | 0   |            |
| C    | 4    | 0   | 60  | Na   | 1    | 0   | 0   | K     | 1    | 0   | 0   |        |      |     |     |            |
| N    | 3    | 0   | 0   | Si   | 4    | 0   | 0   | Mn    | 3    | 0   | 0   |        |      |     |     |            |

Error Margin (ppm): 100
DBE Range: -2.0 - 1000.0
Electron Ions: both

HC Ratio: unlimited
Apply N Rule: yes
Use MSn Info: no

Max Isotopes: all
Isotope RI (%): 1.00
MSn Logic Mode: AND
Max Results: 500

Event#: 1 MS(E+)
Ret. Time: 1.507
Scan#: 227

Measured region for 267.0652 m/z

C16 H10 O4 [M+H]+ : Predicted region for 267.0652 m/z

Rank | Score | Formula (M) | Ion   | Meas. m/z | Pred. m/z | Df. (mDa) | Df. (ppm) | Iso | DBE |
-----|-------|-------------|-------|-----------|-----------|-----------|-----------|-----|-----|
1    | 75.33 | C16 H10 O4  | [M+H]+| 267.0652  | 267.0652  | 0.0       | 0.00      | 75.33| 12.0|
Data File: F:\高分辨数据\Zouyong\sjf\S3.lcd

| Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Elmt | Val. | Min | Max |
|------|------|-----|-----|------|------|-----|-----|------|------|-----|-----|------|------|-----|-----|------|------|-----|-----|
| H    | 1    | 0   | 80  | O    | 2    | 0   | 20  | P    | 3    | 0   | 0   | Zn   | 2    | 0   | 0   | H    | 1    | 0   | 80  |
| 2H   | 1    | 0   | 0   | 18O  | 2    | 0   | 0   | S    | 2    | 0   | 0   | Se   | 2    | 0   | 0   | O    | 2    | 0   | 20  |
| B    | 3    | 0   | 0   | F    | 1    | 0   | 0   | Cl   | 1    | 0   | 0   | Br   | 1    | 0   | 0   | 2H   | 1    | 0   | 0   |
| N    | 4    | 0   | 60  | Na   | 1    | 0   | 0   | K    | 1    | 0   | 0   | Mn   | 3    | 0   | 0   | B    | 3    | 0   | 0   |

Error Margin (ppm): 100  
DBE Range: -2.0 - 1000.0  
Electron Ions: both  
Apply N Rule: yes  
Use MSn Info: no  

HC Ratio: unlimited  
Max Isotopes: all  
Msn Iso RI (%): 75.00  
Msn Logic Mode: AND  
Max Results: 500  

Event#: 1  
M(E+) Ret. Time: 1.480  
Scan#: 223  

Measured region for 297.0756 m/z  
C17 H12 O5 [M+H]+ : Predicted region for 297.0758 m/z

| Rank | Score | Formula (M) | Ion | Meas. m/z | Pred. m/z | Df. (mDa) | Df. (ppm) | Iso | DBE |
|------|-------|-------------|-----|-----------|-----------|-----------|-----------|-----|-----|
| 1    | 72.99 | C17 H12 O5  | [M+H]+ | 297.0756  | 297.0758  | -0.2      | -0.67     | 72.99| 12.0|
### Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Use Adduct
---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---
H  | 1   | 0   | 80  | O  | 2   | 0   | 20  | P  | 3   | 0   | 0  | Zn  | 2   | 0   | 0  | H  
2H | 1   | 0   | 0   | 18O| 2   | 0   | 0   | S  | 2   | 0   | 0  | Se  | 2   | 0   | 0  
B  | 3   | 0   | 0   | F  | 1   | 0   | 0   | Cl | 1   | 0   | 0  | Br  | 1   | 0   | 0  
C  | 4   | 0   | 60  | Na | 1   | 0   | 0   | K  | 1   | 0   | 0  | Mn  | 3   | 0   | 0  
N  | 3   | 0   | 0   | Si | 4   | 0   | 0   |  

Error Margin (ppm): 100  
DBE Range: -2.0 - 1000.0  
Electron Ions: both  
Apply N Rule: yes  
Use MSn Info: no  
Max Isotopes: all  
Isotope RI (%): 75.00  
MSn Iso RI (%): 75.00  
MSn Logic Mode: AND  
Max Results: 500  

#### Event# 1 MS(E+)  Ret. Time : 1.227  Scan# : 185

**Measured region for 327.0854 m/z**

**C18 H14 O6 [M+H]+** : Predicted region for 327.0863 m/z

| Rank | Score | Formula (M) | Ion       | Meas. m/z | Pred. m/z | Df. (mDa) | Df. (ppm) | Iso | DBE |
|------|-------|-------------|-----------|-----------|-----------|-----------|-----------|-----|-----|
| 1    | 75.67 | C18 H14 O6  | [M+H]+    | 327.0854  | 327.0863  | -0.9      | -2.75     | 79.13 | 12.0 |
### Element Table

| Elmt | Val. | Min  | Max  |
|------|------|------|------|
| H    | 1    | 0    | 80   |
| O    | 2    | 0    | 20   |
| P    | 3    | 0    | 0    |
| Zn   | 2    | 0    | 0    |
| H2   | 1    | 0    | 0    |
| 18O  | 2    | 0    | 0    |
| S    | 2    | 0    | 0    |
| Se   | 2    | 0    | 0    |
| B    | 3    | 0    | 0    |
| F    | 1    | 0    | 0    |
| Cl   | 1    | 0    | 0    |
| Br   | 1    | 0    | 0    |
| C    | 4    | 0    | 60   |
| Na   | 1    | 0    | 0    |
| K    | 1    | 0    | 0    |
| Si   | 4    | 0    | 0    |
| Mn   | 3    | 0    | 0    |

### Error Margin (ppm): 100

### DBE Range: -2.0 - 1000.0

### Electron Ions: both

### Apply N Rule: yes

### Use MSn Info: no

### MSn Iso RI (%): 75.00

### MSn Logic Mode: AND

### Max Results: 500

### Event#: 1 MS(E+) Ret. Time : 1.320 Scan#: 199

---

**Error Margin (ppm): 100**

**DBE Range: -2.0 - 1000.0**

**Apply N Rule: yes**

**Use MSn Info: no**

**MSn Iso RI (%): 75.00**

**MSn Logic Mode: AND**

**Max Results: 500**

---

**Event#: 1 MS(E+) Ret. Time : 1.320 Scan#: 199**

---

**C16 H8 O5 [M+H]+ : Predicted region for 281.0444 m/z**

---

**C16 H8 O5 [M+H]+ : Predicted region for 281.0444 m/z**
### Formula Predictor Report - S6.lcd

Data File: F:\高分辨数据\Zouyong\sjf\S6.lcd

| Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Use Adduct |
|------|------|-----|-----|------|------|-----|-----|------|------|-----|-----|------|------|-----|-----|------------|
| H    | 1    | 0   | 80  | O    | 2    | 0   | 20  | P    | 3    | 0   | 0   | Zn   | 2    | 0   | 0   | H          |
| 2H   | 1    | 0   | 0   | 18O  | 2    | 0   | 0   | S    | 2    | 0   | 0   | Se   | 2    | 0   | 0   |            |
| B    | 3    | 0   | 0   | F    | 1    | 0   | 0   | Cl   | 1    | 0   | 0   | Br   | 1    | 0   | 0   |            |
| C    | 4    | 0   | 60  | Na   | 1    | 0   | 0   | K    | 1    | 0   | 0   |        |       |     |     |            |
| N    | 3    | 0   | 0   | Si   | 4    | 0   | 0   | Mn   | 3    | 0   | 0   |        |       |     |     |            |

Error Margin (ppm): 100  
DBE Range: -2.0 - 1000.0  
Electron Ions: both  
Apply N Rule: yes  
Use MSn Info: no  
Max Results: 500

Event#: 1 MS(E+)  
Ret. Time: 1.120  
Scan#: 169

**Measured region for 303.0645 m/z**

**C19 H10 O4 [M+H]+ : Predicted region for 303.0652 m/z**
Data File: F高分辨数据\Zouyong\sjf\S7.lcd

Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Use Adduct
--- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | ---
H   | 1    | 0   | 80  | O    | 2    | 0   | 20  | P    | 3    | 0   | 0   | Zn   | 2    | 0   | 0   | H
2H  | 1    | 0   | 0   | 18O  | 2    | 0   | 0   | S    | 2    | 0   | 0   | Se   | 2    | 0   | 0   |
B   | 3    | 0   | 0   | F    | 1    | 0   | 0   | Cl   | 1    | 0   | 0   | Br   | 1    | 0   | 0   |
C   | 4    | 0   | 60  | Na   | 1    | 0   | 0   | K    | 1    | 0   | 0   |
N   | 3    | 0   | 0   | Si   | 4    | 0   | 0   | Mn   | 3    | 0   | 0   |

Error Margin (ppm): 100
DBE Range: -2.0 - 1000.0
Electron Ions: both
HC Ratio: unlimited
Apply N Rule: yes
Max Isotopes: all
Isotope RI (%): 1.00
MSn Info: no
Mn Logic Mode: AND
Max Results: 500

Event#: 1 MS(E+)
Ret. Time: 1.213
Scan#: 183

Measured region for 253.0493 m/z

C15 H8 O4 [M+H]+: Predicted region for 253.0495 m/z

Rank | Score | Formula (M) | Ion | Meas. m/z | Pred. m/z | Df. (mDa) | Df. (ppm) | Iso | DBE
--- | --- | --- | --- | --- | --- | --- | --- | --- | ---
1 | 77.50 | C15 H8 O4 | [M+H]+ | 253.0495 | 253.0495 | -0.2 | -0.79 | 77.50 | 12.0
Data File: FA高分辨数据/Zouyong/sjf/S8.lcd

| Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Use Adduct |
|------|------|-----|-----|------|------|-----|-----|------|------|-----|-----|------|------|-----|-----|------|------|-----|-----|-------------|
| H    | 1    | 0   | 80  | O    | 2    | 0   | 20  | P    | 3    | 0   | 0   | Zn   | 2    | 0   | 0   | H    | 1    | 0   | 80  | 1i           |
| 2H   | 1    | 0   | 0   | 18O  | 2    | 0   | 0   | S    | 2    | 0   | 0   | Se   | 2    | 0   | 0   | 2H   | 1    | 0   | 0   |              |
| B    | 3    | 0   | 0   | F    | 1    | 0   | 0   | Cl   | 1    | 0   | 0   | Br   | 1    | 0   | 0   | B    | 3    | 0   | 0   |              |
| C    | 4    | 0   | 60  | Na   | 1    | 0   | 0   | K    | 1    | 0   | 0   | Mn   | 3    | 0   | 0   | C    | 4    | 0   | 60  |              |

Error Margin (ppm): 100
DBE Range: -2.0 - 1000.0
Electron Ions: both
Apply N Rule: yes
Use MSn Info: no
Max Isotopes: all
MSn Iso RI (%): 75.00
MSn Logic Mode: AND
Max Results: 500

Event#: 1 MS(E+) Ret. Time: 1.227 Scan#: 185

Measured region for 283.0595 m/z

C16 H10 O5 [M+H]+ : Predicted region for 283.0601 m/z

Rank  Score  Formula (M)  Ion  Meas. m/z  Pred. m/z  Df. (mDa)  Df. (ppm)  Iso  DBE
1  78.97  C16 H10 O5  [M+H]+  283.0595  283.0601  -0.6  -2.12  81.24  12.0
### Data File: F:\高分辨数据\Zouyong\sjf\S9.lcd

#### Element Table

| Elmt | Val. | Min | Max |
|------|------|-----|-----|
| H    | 1    | 0   | 80  |
| O    | 2    | 0   | 20  |
| P    | 3    | 0   | 0   |
| Zn   | 2    | 0   | 0   |
| B    | 3    | 0   | 0   |
| F    | 1    | 0   | 0   |
| Si   | 4    | 0   | 0   |
| Na   | 1    | 0   | 0   |
| K    | 1    | 0   | 0   |
| Mn   | 3    | 0   | 0   |
| C    | 4    | 0   | 60  |

#### Use Adduct

- **Use Adduct**: H
- **Electron Ions**: both
- **Apply N Rule**: yes
- **Use MSn Info**: no
- **Max Isotopes**: all
- **MSn Iso RI (%)**: 75.00
- **MSn Logic Mode**: AND
- **Max Results**: 500
- **Error Margin (ppm)**: 100
- **DBE Range**: -2.0 - 1000.0
- **HC Ratio**: unlimited

#### Measured region for 343.0803 m/z

![Measured region graph](image_url)

#### Predicted region for 343.0812 m/z

![Predicted region graph](image_url)

### Event 

- **Event #: 1 MS(E+) Ret. Time : 1.133 Scan #: 171**

#### C18 H14 O7 [M+H]+ : Predicted region for 343.0812 m/z

| Rank | Score | Formula (M) | Ion | Meas. m/z | Pred. m/z | Df. (mDa) | Df. (ppm) | Iso | DBE |
|------|-------|-------------|-----|-----------|-----------|-----------|-----------|-----|-----|
| 1    | 71.06 | C18 H14 O7  | [M+H]+ | 343.0803  | 343.0812  | -0.9      | -2.62     | 74.06| 12.0|
Data File: \Deep-20160624\data1\SXH\SJF-1K.lcd

| Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Elmt | Val. | Min | Max |
|------|------|-----|-----|------|------|-----|-----|------|------|-----|-----|
| H    | 1    | 6   | 10  | O    | 2    | 2   | 3   | K    | 1    | 0   | 0   |
| 2H   | 1    | 0   | 0   | F    | 1    | 0   | 0   | Mn   | 3    | 0   | 0   |
| 3H   | 1    | 0   | 0   | Si   | 4    | 0   | 0   | Fe   | 2    | 0   | 0   |
| B    | 3    | 0   | 0   | P    | 3    | 0   | 0   | Cu   | 2    | 0   | 0   |
| C    | 4    | 14  | 16  | S    | 2    | 0   | 0   | Se   | 2    | 0   | 0   |
| N    | 3    | 0   | 0   | Cl   | 1    | 0   | 0   | Br   | 1    | 0   | 0   |

Error Margin (ppm): 100
HC Ratio: 0.0 - 100.0
Max Isotopes: all
MSn Iso RI (%): 75.00
MSn Logic Mode: AND
Max Results: 100

Event#: 1 MS(E+)  Ret. Time: 1.320 -> 1.320  Scan#: 199 -> 199

Measured region for 251.0701 m/z

C16 H10 O3 [M+H]+ : Predicted region for 251.0703 m/z
Event#: 1 MS(E+)   Ret. Time : 1.560   Scan# : 235

| Elmt | Val. | Min | Max |
|------|------|-----|-----|
| H    | 1    | 0   | 80  |
| 2H   | 1    | 0   | 0   |
| B    | 3    | 0   | 0   |
| C    | 4    | 0   | 60  |
| N    | 3    | 0   | 0   |

| Elmt | Val. | Min | Max |
|------|------|-----|-----|
| O    | 2    | 0   | 20  |
| 18O  | 2    | 0   | 0   |
| F    | 1    | 0   | 0   |
| Na   | 1    | 0   | 0   |
| Si   | 4    | 0   | 0   |

Elmt | Val. | Min | Max | Use Adduct
-----|------|-----|-----|-----------------
P    | 3    | 0   | 0   | H
S    | 2    | 0   | 0   | 18O
Cl   | 1    | 0   | 0   | F
K    | 1    | 0   | 0   | Na
Mn   | 3    | 0   | 0   | Si

Error Margin (ppm): 100
HC Ratio: unlimited
Max Isotopes: all
MSn Iso RI (%): 75.00
MSn Logic Mode: AND
Max Results: 500

Electron Ions: both
Apply N Rule: yes
Use MSn Info: no
Isotope Res: 10000
Isotope RI (%): 1.00
DBE Range: -2.0 - 1000.0

Event: #1 MS(E+), Ret. Time: 1.560, Scan#: 235

C16 H10 O4 [M+H]+ : Predicted region for 267.0652 m/z
Data File: F高分辨数据\Zouyong\sjf\S15.lcd

| Elmt | Val. | Min | Max |
|------|------|-----|-----|
| H    | 1    | 0   | 80  |
| 2H   | 1    | 0   | 0   |
| B    | 3    | 0   | 0   |
| C    | 4    | 0   | 60  |
| N    | 3    | 0   | 0   |
| O    | 2    | 0   | 20  |
| P    | 3    | 0   | 0   |
| S    | 2    | 0   | 0   |
| Se   | 2    | 0   | 0   |
| Br   | 1    | 0   | 0   |
| Cl   | 1    | 1   | 1   |
| F    | 1    | 0   | 0   |
| Na   | 1    | 0   | 0   |
| K    | 1    | 0   | 0   |
| Mn   | 3    | 0   | 0   |

Use Adduct: H

Error Margin (ppm): 100
DBE Range: -2.0 - 1000.0
Electron Ions: both
Max Isotopes: all
MSn_logic Mode: AND
Max Results: 500

Event#: 1 MS(E+)
Ret. Time : 1.680
Scan#: 253

Measured region for 271.0156 m/z

C15 H7 O3 Cl [M+H]⁺: Predicted region for 271.0156 m/z
Data File: F:\高分辨数据\Zouyong\sjf\S11.lcd

| Elmt | Val. | Min | Max |
|------|------|-----|-----|
| H    | 1    | 0   | 80  |
| O    | 2    | 0   | 20  |
| P    | 3    | 0   | 0   |
| Zn   | 2    | 0   | 0   |
| N    | 3    | 0   | 60  |
| Si   | 4    | 0   | 0   |

Error Margin (ppm): 100
DBE Range: -2.0 - 1000.0
Electron Ions: both
Apply N Rule: yes
Use MSn Info: no
Max Isotopes: all
Isotope RI (%): 75.00
MSn Logic Mode: AND
Max Results: 500

Event#: 1 MS(E+) Ret. Time: 1.360 Scan#: 205

Measured region for 283.0598 m/z

C16 H10 O5 [M+H]+: Predicted region for 283.0601 m/z
# Formula Predictor Report - S12.lcd

Data File: F:\高分辨数据\Zouyong\sjf\S12.lcd

| Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Use Adduct |
|------|------|-----|-----|------|------|-----|-----|------|------|-----|-----|------|------|-----|-----|-------------|
| H    | 1    | 0   | 80  | O    | 2    | 0   | 20  | P    | 3    | 0   | 0   | Zn   | 2    | 0   | 0   | H           |
| 2H   | 1    | 0   | 0   | 18O  | 2    | 0   | 0   | S    | 2    | 0   | 0   | Se   | 2    | 0   | 0   |             |
| B    | 3    | 0   | 0   | F    | 1    | 0   | 0   | Cl   | 1    | 0   | 0   | Br   | 1    | 0   | 0   |             |
| N    | 3    | 0   | 60  | Na   | 1    | 0   | 0   | K    | 1    | 0   | 0   | Mn   | 3    | 0   | 0   |             |

Error Margin (ppm): 100
DBE Range: -2.0 - 1000.0
Electron Ions: both
Max Isotopes: all
MSn Iso RI (%): 75.00
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND
Use MSn Info: no
Isotope Res: 10000
Max Results: 500

Event#: 1 MS(E+) Ret. Time : 1.280 Scan#: 193

---

**Measured region for 327.0861 m/z**

**C18 H14 O6 [M+H]+ : Predicted region for 327.0863 m/z**

| Rank | Score | Formula (M) | Ion     | Meas. m/z | Pred. m/z | Df. (mDa) | Df. (ppm) | Iso | DBE |
|------|-------|-------------|---------|-----------|-----------|-----------|-----------|-----|-----|
| 1    | 80.48 | C18 H14 O6  | [M+H]+  | 327.0861  | 327.0863  | -0.2      | -0.61     | 80.48| 12.0|
Data File: \Zouyong\sjf\S13.lcd

| Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Use Adduct |
|------|------|-----|-----|------|------|-----|-----|------|------|-----|-----|------|------|-----|-----|------------|
| H    | 1    | 0   | 80  | O    | 2    | 0   | 20  | P    | 3    | 0   | 0   | Zn   | 2    | 0   | 0   | H          |
| 2H   | 1    | 0   | 0   | 18O  | 2    | 0   | 0   | S    | 2    | 0   | 0   | Se   | 2    | 0   | 0   |            |
| B    | 3    | 0   | 0   | F    | 1    | 0   | 0   | Cl   | 1    | 0   | 0   | Br   | 1    | 0   | 0   |            |
| C    | 4    | 0   | 60  | Na   | 1    | 0   | 0   | K    | 1    | 0   | 0   |       |      |     |     |            |
| N    | 3    | 0   | 0   | Si   | 4    | 0   | 0   | Mn   | 3    | 0   | 0   |       |      |     |     |            |

Error Margin (ppm): 100
DBE Range: -2.0 - 1000.0
Electron Ions: both
Apply N Rule: yes
Use MSn Info: no
Max Isotopes: all
MSn Iso RI (%): 75.00
MSn Logic Mode: AND
Max Results: 500

Event#: 1 MS(E+), Ret. Time: 1.307, Scan#: 197

Measured region for 357.0964 m/z

C19 H16 O7 [M+H]+: Predicted region for 357.0969 m/z
Data File: F:\高分辨数据\Zouyong\sjf\S14.lcd

| Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Use Adduct |
|------|------|-----|-----|------|------|-----|-----|------|------|-----|-----|------------|
| H    | 1    | 0   | 80  | O    | 2    | 0   | 20  | P    | 3    | 0   | 0   |            |
| 2H   | 1    | 0   | 0   | 18O  | 2    | 0   | 0   | S    | 2    | 0   | 0   |            |
| B    | 3    | 0   | 0   | F    | 1    | 0   | 0   | Cl   | 1    | 0   | 0   |            |
| C    | 4    | 0   | 60  | Na   | 1    | 0   | 0   | K    | 1    | 0   | 0   |            |
| N    | 3    | 0   | 0   | Si   | 4    | 0   | 0   | Mn   | 3    | 0   | 0   | H          |

Error Margin (ppm): 100  DBE Range: -2.0 - 1000.0  Electron Ions: both
Max Isotopes: all  Isotope RI (%): 1.00  Use MSn Info: no
HC Ratio: unlimited  Isotope Res: 10000  Max Results: 500
Apply N Rule: yes  MSn Iso RI (%): 75.00  MSn Logic Mode: AND

Event#: 1 MS(E+)  Ret. Time: 1.693  Scan#: 255

Measured region for 297.0756 m/z

C17 H12 O5 [M+H]+ : Predicted region for 297.0758 m/z

| Rank | Score | Formula (M) | Ion   | Meas. m/z | Pred. m/z | Df. (mDa) | Df. (ppm) | Iso | DBE |
|------|-------|-------------|-------|-----------|-----------|-----------|-----------|-----|-----|
| 1    | 74.57 | C17 H12 O5  | [M+H]+| 297.0756  | 297.0758  | -0.2      | -0.67     | 74.57| 12.0|
Data File: \Deep-20160624ld\data1\邹永\SXH\SJF-1R.lcd

| Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Use Adduct |
|------|------|-----|-----|------|------|-----|-----|------|------|-----|-----|------|------|-----|-----|------|------|-----|-----|-------------|
| H    | 1    | 14  | 16  | O    | 2    | 5   | 8   | K    | 1    | 0   | 0   | Pd   | 2    | 0   | 0   | H    | 1    | 0   | 0   |-------------|
| 2H   | 1    | 0   | 0   | F    | 1    | 0   | 0   | Mn   | 3    | 0   | 0   | I    | 3    | 0   | 0   | Na   | 1    | 0   | 0   |-------------|
| 3H   | 1    | 0   | 0   | Si   | 4    | 0   | 0   | Fe   | 2    | 0   | 0   | Pt   | 2    | 0   | 0   | H    | 1    | 0   | 0   |-------------|
| B    | 3    | 0   | 0   | P    | 3    | 0   | 0   | Cu   | 2    | 0   | 0   | Au   | 1    | 0   | 0   | Au   | 1    | 0   | 0   |-------------|
| C    | 4    | 0   | 0   | Cl   | 1    | 0   | 0   | Se   | 2    | 0   | 0   | Br   | 1    | 0   | 0   | Br   | 1    | 0   | 0   |-------------|

Error Margin (ppm): 100
HC Ratio: 0.0 - 100.0
Max Isotopes: all
MSn Iso RI (%): 75.00
MSn Logic Mode: AND
Max Results: 100

Event#: 1 MS(E+)   Ret. Time : 1.040 -> 1.040   Scan# : 157 -> 157

Measured region for 357.0965 m/z

C19 H16 O7 [M+H]+: Predicted region for 357.0969 m/z
Data File: \Deep-20160624\data1\XHX\SJF-1S.lcd

| Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Use Adduct |
|------|------|-----|-----|------|------|-----|-----|------|------|-----|-----|------|------|-----|-----|------------|
| H    | 1    | 6   | 8   | O    | 2    | 4   | 5   | K    | 1    | 0   | 0   | Pd   | 2    | 0   | 0   | H          |
| 2H   | 1    | 0   | 0   | F    | 1    | 0   | 0   | Mn   | 3    | 0   | 0   | I    | 3    | 0   | 0   | Na         |
| 3H   | 1    | 0   | 0   | Si   | 4    | 0   | 0   | Fe   | 2    | 0   | 0   | Pt    | 2    | 0   | 0   |            |
| B    | 3    | 0   | 0   | P    | 3    | 0   | 0   | Cu   | 2    | 0   | 0   | Au    | 1    | 0   | 0   |            |
| C    | 4    | 14  | 15  | Cl   | 1    | 0   | 0   | Se   | 2    | 0   | 0   |            |      |     |     |            |
| N    | 3    | 0   | 0   | Si   | 4    | 0   | 0   | Fe   | 2    | 0   | 0   | Pt    | 2    | 0   | 0   |            |

Error Margin (ppm): 100
HC Ratio: 0.0 - 100.0
DBE Range: -100.0 - 200.0
Max Isotopes: all
Electron Ions: both
Isotope RI (%): 1.00
Use MSn Info: no
Isotope Res: 10000
MSn Logic Mode: AND
Max Results: 100
Apply N Rule: yes

Event#: 1 MS(E+) Ret. Time: 0.800 -> 0.800 Scan#: 121 -> 121
Data File: F:
Zouyong\sjf\S16.lcd

| Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Elmt | Val. | Min | Max |
|------|------|-----|-----|------|------|-----|-----|------|------|-----|-----|------|------|-----|-----|
| H    | 1    | 0   | 80  | O    | 2    | 0   | 20  | P    | 3    | 0   | 0   | H    | 3    | 0   | 0   |
| 2H   | 1    | 0   | 0   | 18O  | 2    | 0   | 0   | S    | 2    | 0   | 0   | Se   | 2    | 0   | 0   |
| B    | 3    | 0   | 0   | F    | 1    | 0   | 0   | Cl   | 1    | 0   | 0   | Br   | 1    | 0   | 0   |
| C    | 60   | 4   | 0   | Na   | 1    | 0   | 0   | K    | 1    | 0   | 0   | Si   | 4    | 0   | 0   |

Use Adduct:

Error Margin (ppm): 100
DBE Range: -2.0 - 1000.0
Electron Ions: both
Apply N Rule: yes
Use MSn Info: no
HC Ratio: unlimited
Max Isotopes: all
MSn Iso RI (%): 75.00
MSn Logic Mode: AND
Max Results: 500

Event#: 1 MS(E+)  Ret. Time : 1.333  Scan#: 201

C16 H10 O5 [M+H]+ : Predicted region for 283.0601 m/z
Data File: F:\高分辨数据\Zouyong\sjf\S17.lcd

| Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Use Adduct |
|------|------|-----|-----|------|------|-----|-----|------|------|-----|-----|-------------|
| H    | 1    | 0   | 80  | O    | 2    | 0   | 20  | P    | 3    | 0   | 0   | H           |
| 2H   | 1    | 0   | 0   | 18O  | 2    | 0   | 0   | S    | 2    | 0   | 0   |             |
| B    | 3    | 0   | 0   | F    | 1    | 0   | 0   | Cl   | 1    | 0   | 0   |             |
| C    | 4    | 0   | 60  | Na   | 1    | 0   | 0   | K    | 1    | 0   | 0   |             |
| N    | 3    | 0   | 0   | Si   | 4    | 0   | 0   | Mn   | 3    | 0   | 0   |             |

Error Margin (ppm): 100  
DBE Range: -2.0 - 1000.0  
Electron Ions: both

HC Ratio: unlimited  
Apply N Rule: yes  
Use MSn Info: no

Max Isotopes: all  
Isotope RI (%): 1.00  
MSn Logic Mode: AND

Max Results: 500

Event#: 1 MS(E+)  Ret. Time: 1.240  Scan#: 187

Measured region for 313.0704 m/z

C17 H12 O6 [M+H]+: Predicted region for 313.0707 m/z

| Rank | Score | Formula (M) | Ion     | Meas. m/z | Pred. m/z | Df. (mDa) | Df. (ppm) | Iso | DBE |
|------|-------|-------------|---------|-----------|-----------|-----------|-----------|-----|-----|
| 1    | 86.34 | C17 H12 O6  | [M+H]+  | 313.0704  | 313.0707  | -0.3      | -0.96     | 86.34| 12.0|
Data File: 高分辨数据\Zouyong\sjf\S18.lcd

Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Use Adduct
--- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | ---
H   | 1   | 0   | 80  | O    | 2   | 0   | 20  | P    | 3   | 0   | 0   | H
2H  | 1   | 0   | 0   | 18O | 2   | 0   | 0   | S    | 2   | 0   | 0   | 1
B   | 3   | 0   | 0   | F    | 1   | 0   | 0   | Cl   | 1   | 0   | 0   | Br
C   | 4   | 0   | 60  | Na   | 1   | 0   | 0   | K    | 1   | 0   | 0   | Si
N   | 3   | 0   | 0   | Si   | 4   | 0   | 0   | Mn   | 3   | 0   | 0   |

Error Margin (ppm): 100
DBE Range: -2.0 - 1000.0
Electron Ions: both
HC Ratio: unlimited
Max Isotopes: all
MSn Iso RI (%): 75.00
MSn Logic Mode: AND
Max Results: 500

Event#: 1 MS(E+)  Ret. Time : 1.200  Scan# : 181

Measured region for 297.0391 m/z

C16 H8 O6 [M+H]⁺: Predicted region for 297.0394 m/z
### Formula Predictor Report - S19.lcd

**Data File:** F:\高分辨数据\Zouyong\sjf\S19.lcd

| Elmt | Val. | Min | Max |
|------|------|-----|-----|
| H    | 1    | 0   | 80  |
| 2H   | 1    | 0   | 0   |
| B    | 3    | 0   | 0   |
| C    | 4    | 0   | 60  |
| N    | 3    | 0   | 0   |
| P    | 3    | 0   | 0   |
| O    | 2    | 0   | 20  |
| S    | 2    | 0   | 0   |
| Se   | 2    | 0   | 0   |
| Cl   | 1    | 0   | 0   |
| Br   | 1    | 0   | 0   |
| F    | 1    | 0   | 0   |
| Na   | 0    | 0   | 0   |
| N    | 3    | 0   | 0   |
| Si   | 4    | 0   | 0   |
| Mn   | 3    | 0   | 0   |

**Use Adduct:**

| Use Adduct | H |
|------------|---|

**Error Margin (ppm):** 100

**DBE Range:** -2.0 - 1000.0

**Electron Ions:** both

**Apply N Rule:** yes

**Use MSn Info:** no

**Max Results:** 500

**Max Isotopes:** all

**Mass Isotope Ratio:** 75.00

**MSn Logic Mode:** AND

**HC Ratio:** unlimited

**Isootope R/%:** 1.00

**M/Res:** 10000

**Event#: 1 MS(E+)  Ret. Time : 1.413  Scan#: 213**

---

**Measured region for 311.0550 m/z**

**C17 H10 O6 [M+H]+ : Predicted region for 311.0550 m/z**
### Table

| Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Elmt | Val. | Min | Max |
|------|------|-----|-----|------|------|-----|-----|------|------|-----|-----|------|------|-----|-----|
| H    | 1    | 0   | 80  | O    | 2    | 0   | 20  | P    | 3    | 0   | 0   | Zn   | 2    | 0   | 0   |
| 2H   | 1    | 0   | 0   | 18O  | 2    | 0   | 0   | S    | 2    | 1   | 1   | Se   | 2    | 0   | 0   |
| B    | 3    | 0   | 0   | F    | 1    | 0   | 0   | Cl   | 1    | 0   | 0   | Br   | 1    | 0   | 0   |
| C    | 4    | 0   | 0   | Na   | 1    | 0   | 0   | K    | 1    | 0   | 0   | Mn   | 3    | 0   | 0   |
| N    | 3    | 0   | 0   | Si   | 4    | 0   | 0   |  

### Error Margin (ppm): 100
- DBE Range: -2.0 - 1000.0
- Electron Ions: both
- Apply N Rule: yes
- Use MSn Info: no
- Isotope RI (%): 1.00
- Isotope Res: 10000
- MSn Logic Mode: AND
- Max Results: 500

### Event#
- 1 MS(E+), Ret. Time: 1.240, Scan#: 187

- Measured region for 403.0853 m/z
- Predicted region for 403.0846 m/z