

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

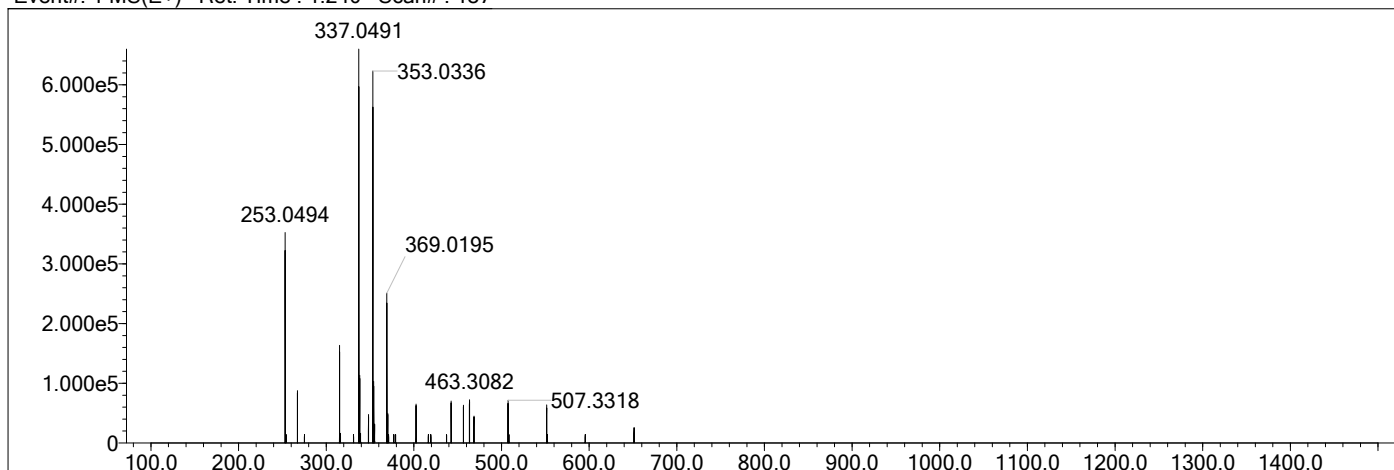
Error Margin (ppm): 100
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

DBE Range: -2.0 - 1000.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

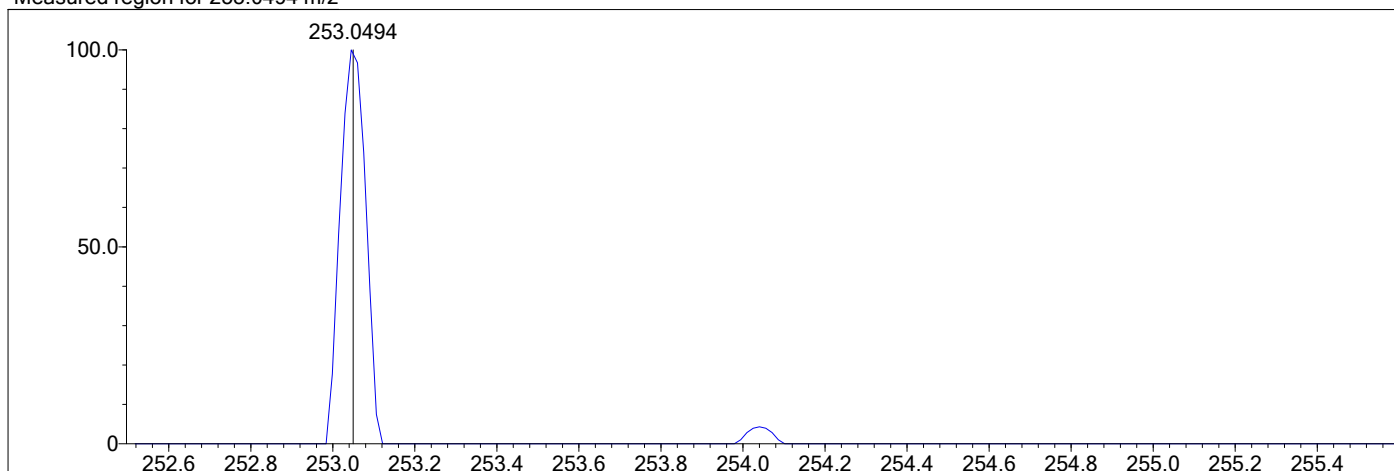
Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

1a

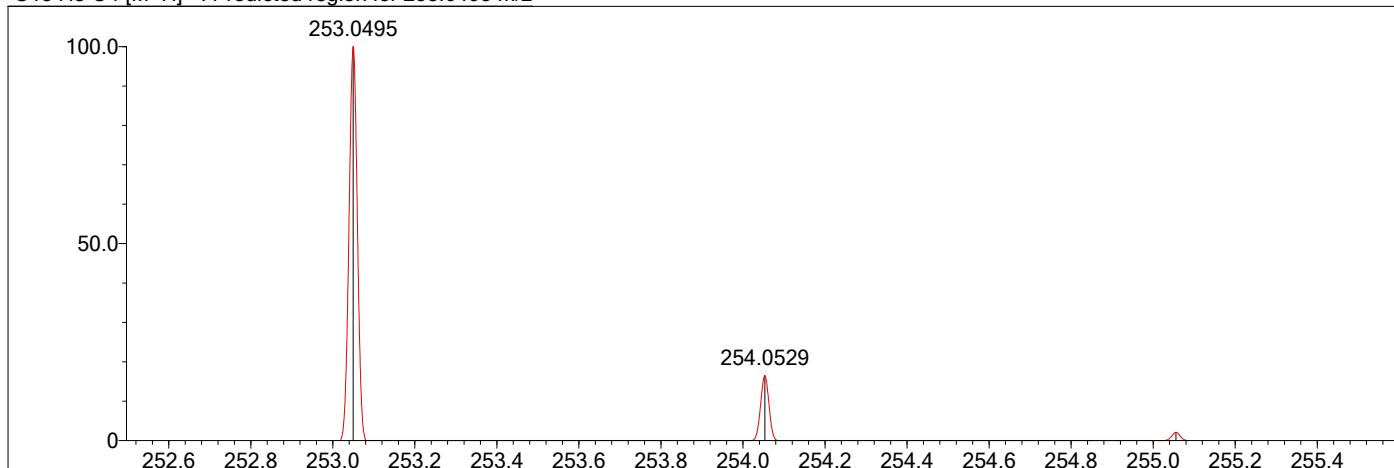
Event#: 1 MS(E+) Ret. Time : 1.240 Scan# : 187



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

Data File: \\Deep-20160624Id\data1\邹永\SXH\SJF-1B.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	2	3	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	S	2	0	0	Se	2	0	0					
N	3	0	0	Cl	1	0	0	Br	1	0	0					

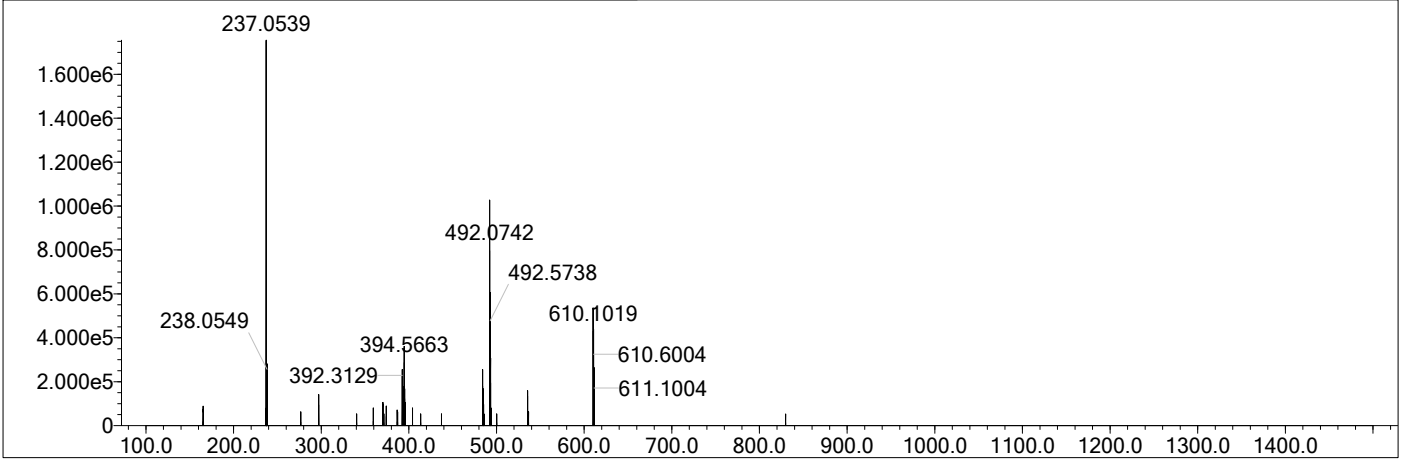
Error Margin (ppm): 100
 HC Ratio: 0.0 - 100.0
 Max Isotopes: all
 MSn Iso RI (%): 75.00

DBE Range: -100.0 - 200.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

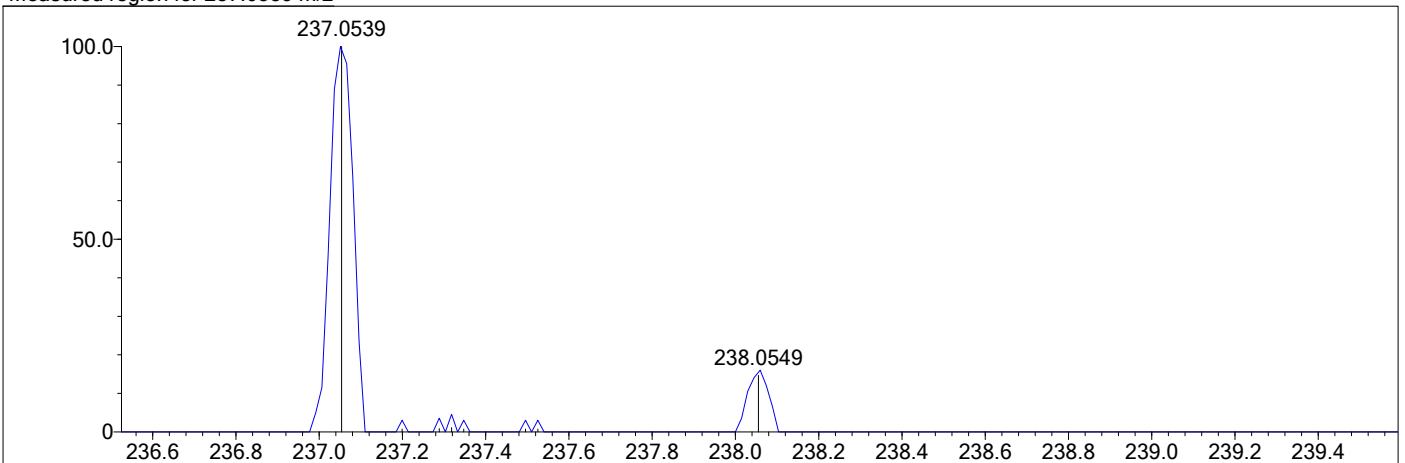
Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 100

1b

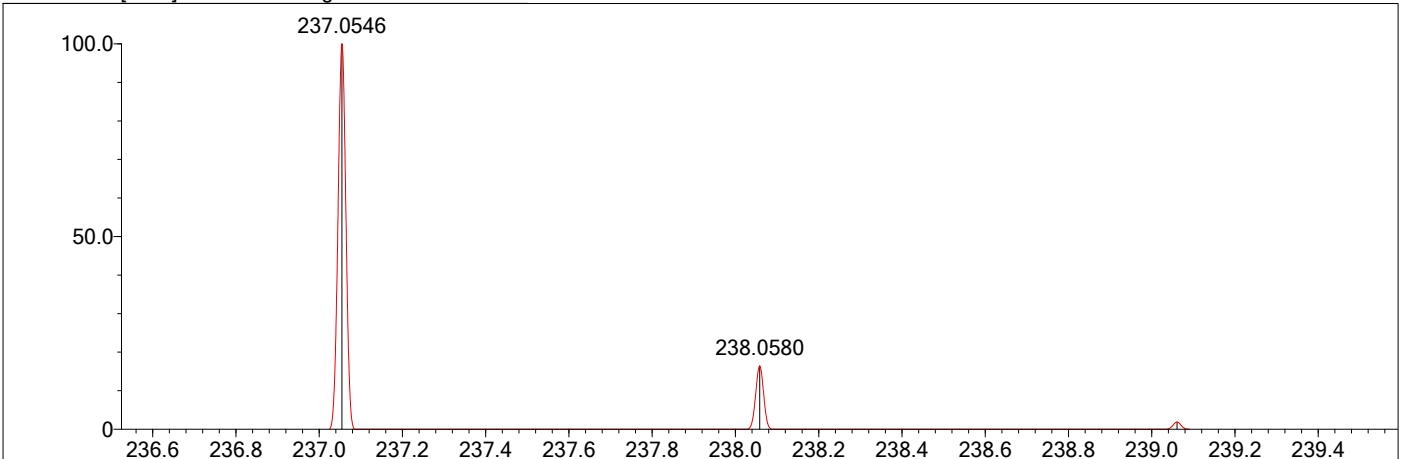
Event#: 1 MS(E+) Ret. Time : 1.120 -> 1.120 Scan# : 169 -> 169



Measured region for 237.0539 m/z



C15 H8 O3 [M+H]+ : Predicted region for 237.0546 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	79.22	C15 H8 O3	[M+H]+	237.0539	237.0546	-0.7	-2.95	83.28	12.0

Data File: F:\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					

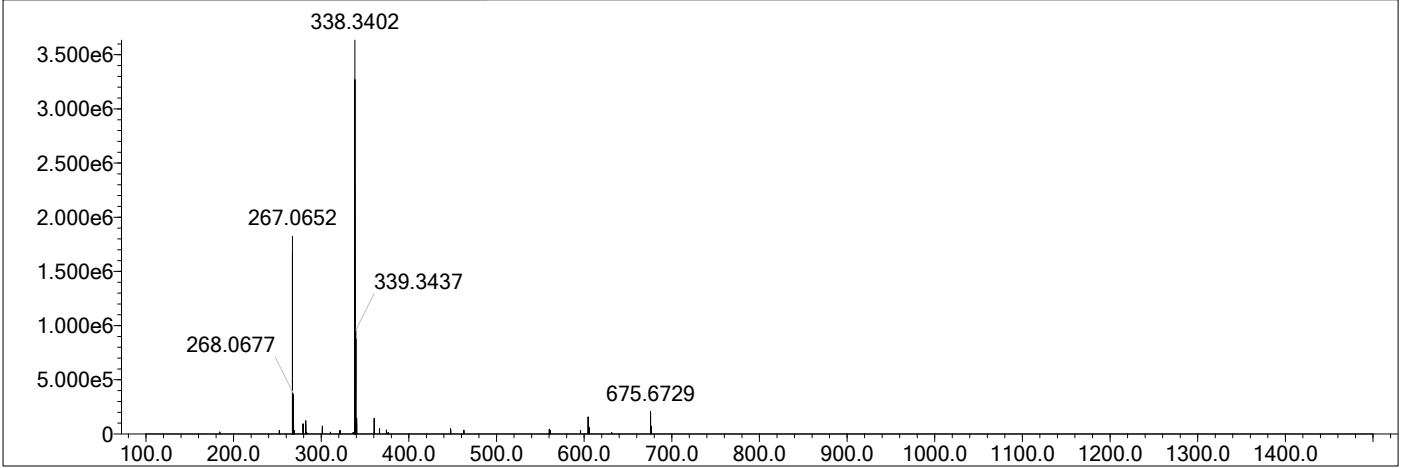
Error Margin (ppm): 100
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

DBE Range: -2.0 - 1000.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

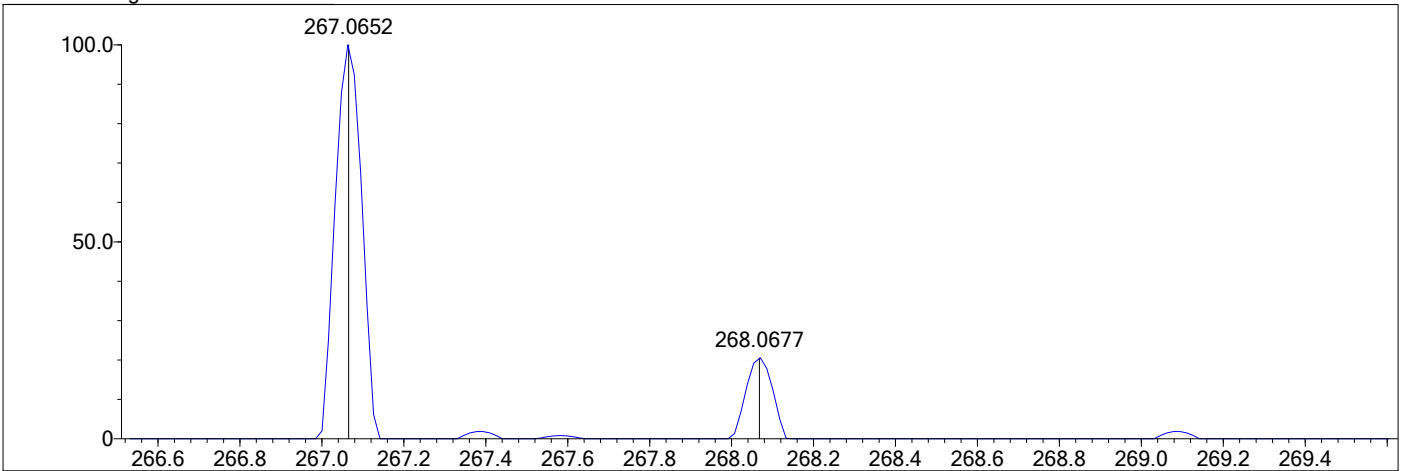
Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

1c

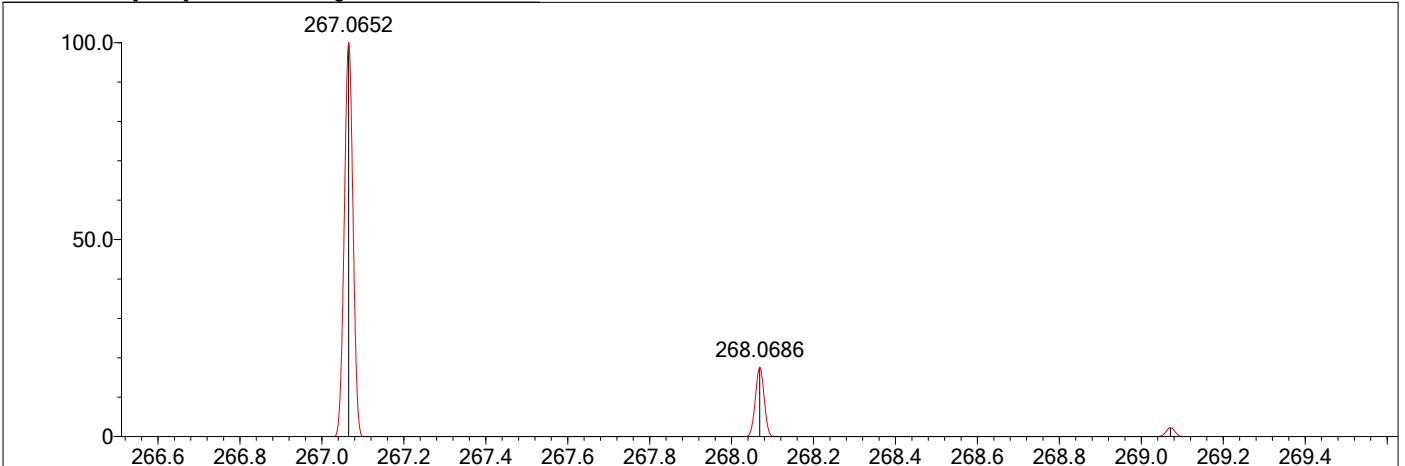
Event#: 1 MS(E+) Ret. Time : 1.507 Scan# : 227



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	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					

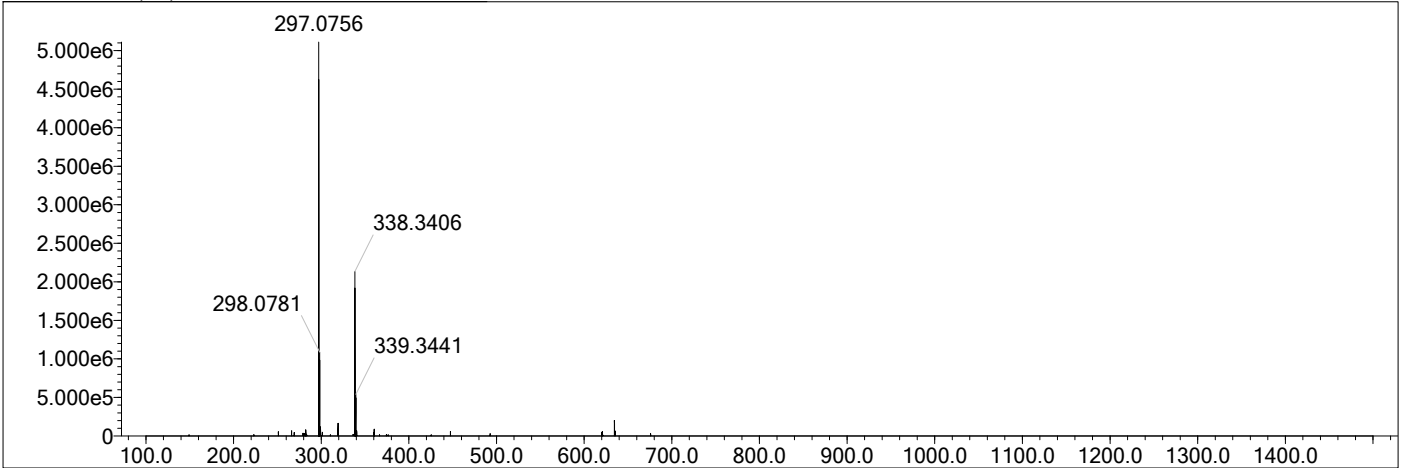
Error Margin (ppm): 100
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

DBE Range: -2.0 - 1000.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

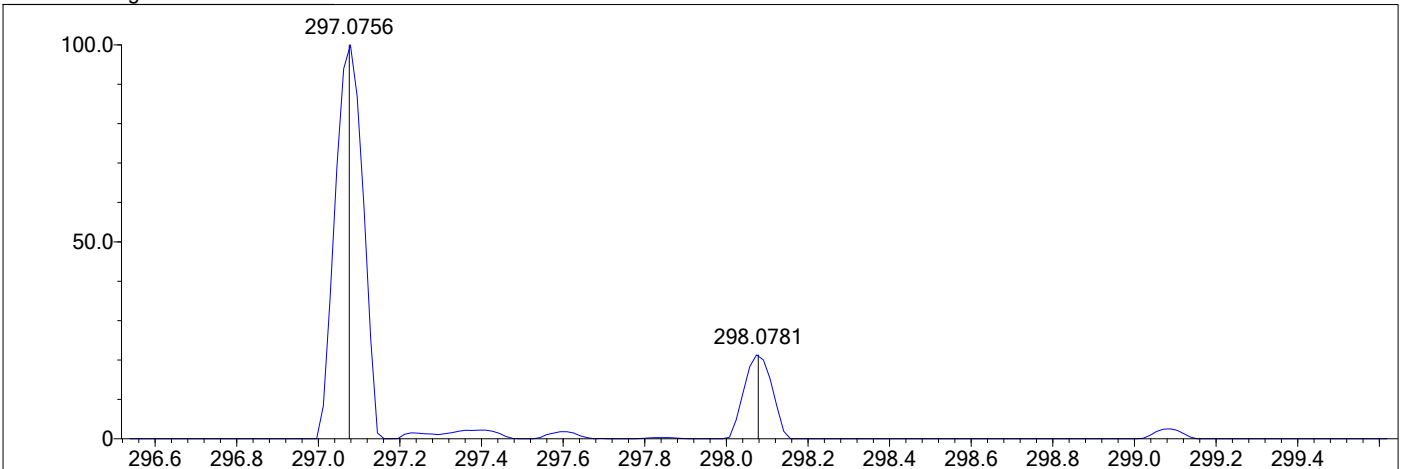
Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

1d

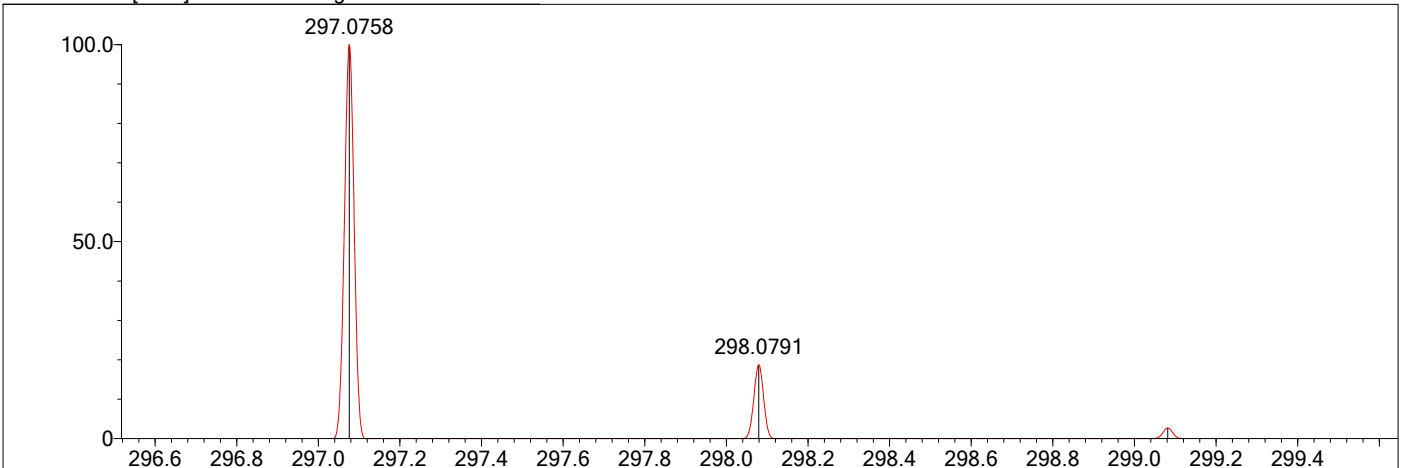
Event#: 1 MS(E+) Ret. Time : 1.480 Scan# : 223



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

Data File: F:\高分辨数据\Zouyong\sjf\S4.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					

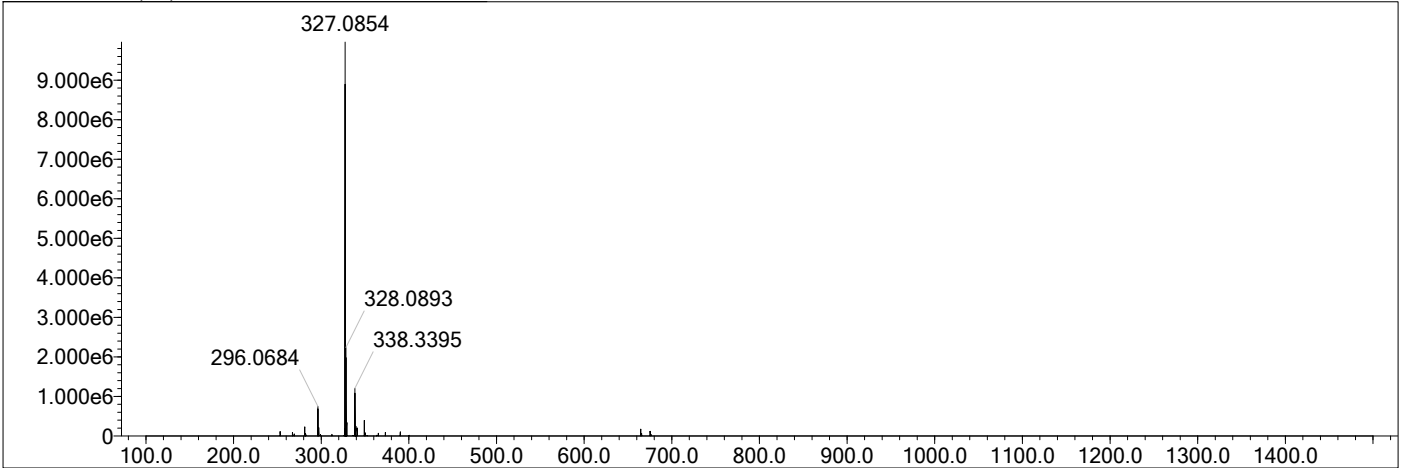
Error Margin (ppm): 100
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

DBE Range: -2.0 - 1000.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

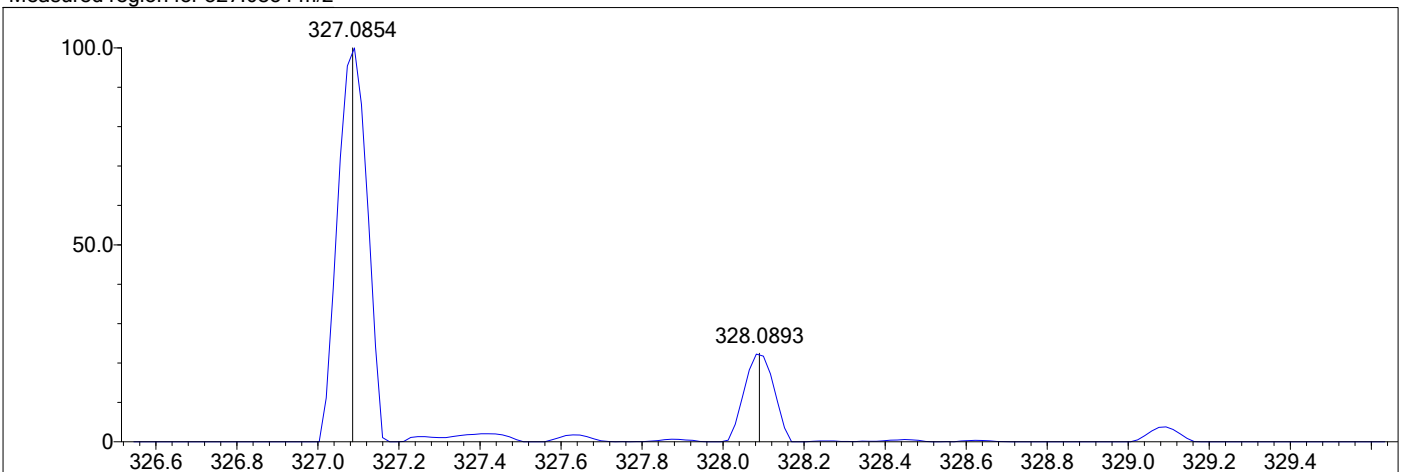
Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

1e

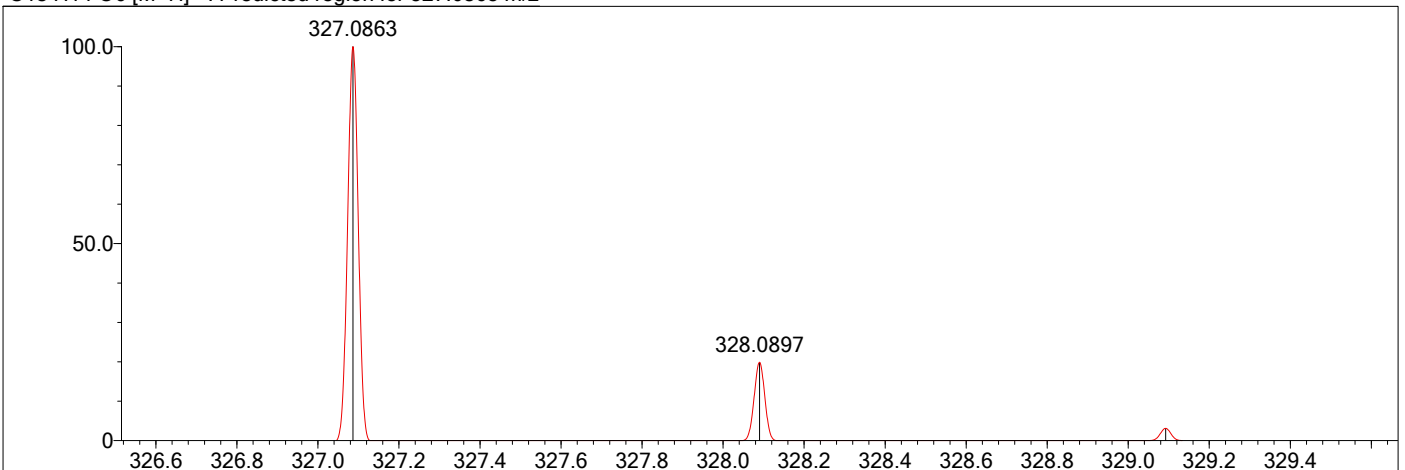
Event#: 1 MS(E+) Ret. Time : 1.227 Scan# : 185



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

Data File: F:\高分辨数据\Zouyong\sjf\S5.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					

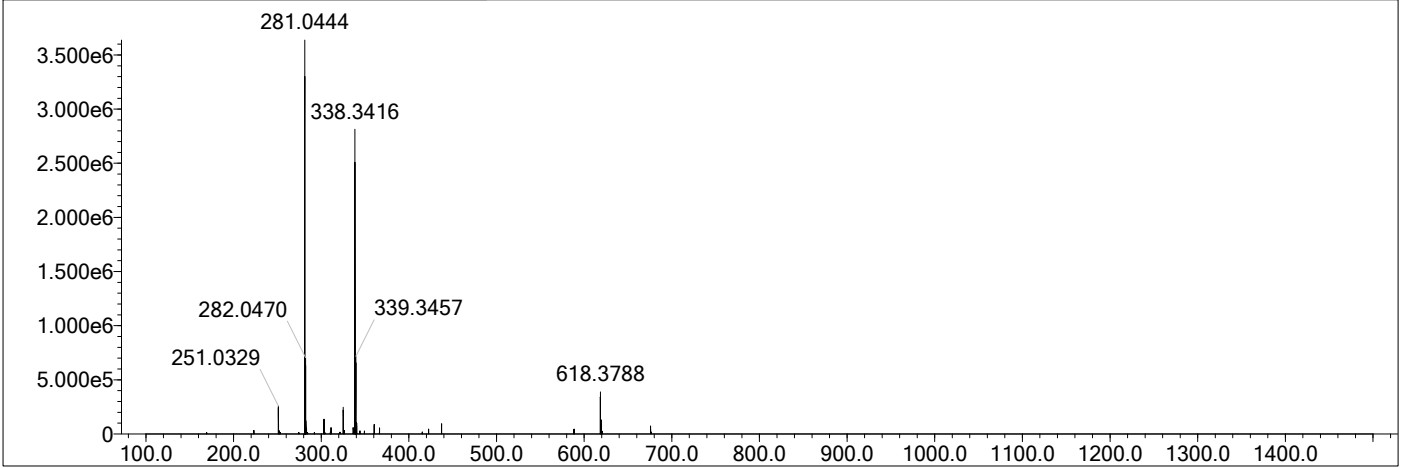
Error Margin (ppm): 100
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

DBE Range: -2.0 - 1000.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

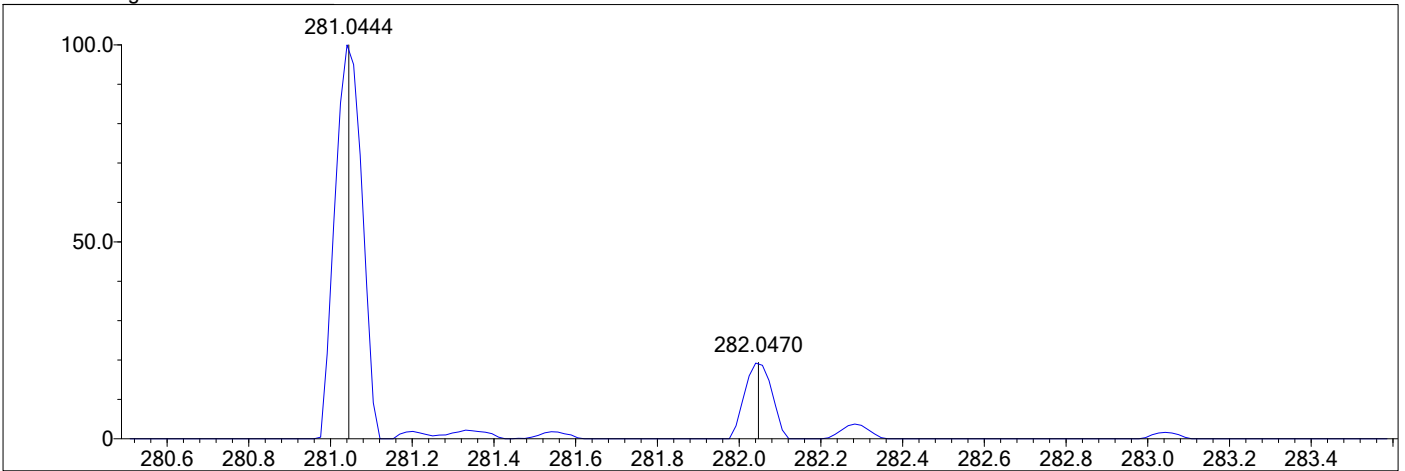
Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

1f

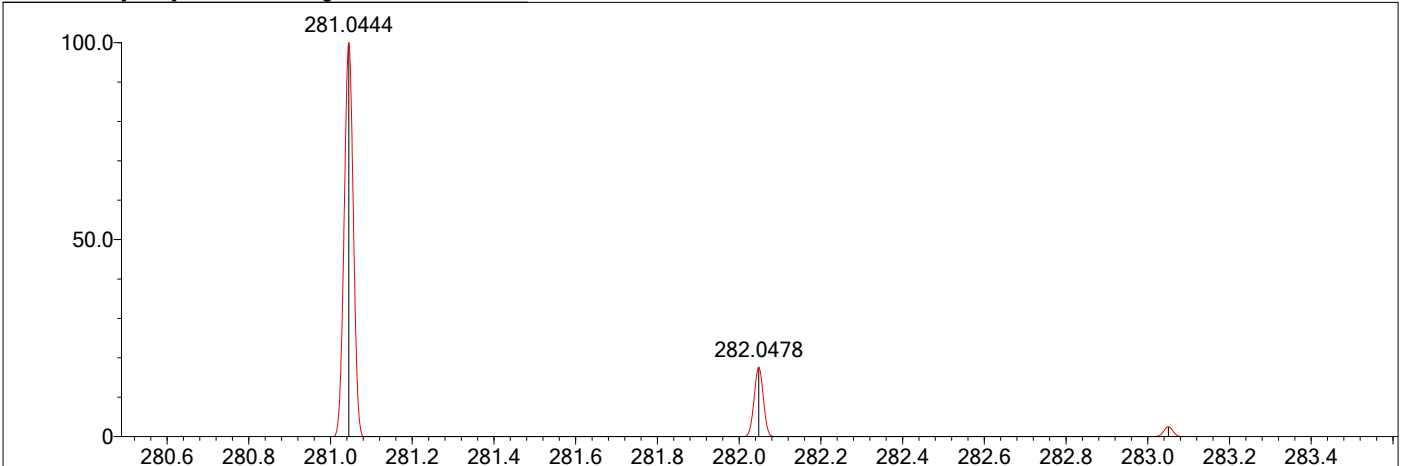
Event#: 1 MS(E+) Ret. Time : 1.320 Scan# : 199



Measured region for 281.0444 m/z



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



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	73.27	C16 H8 O5	[M+H] ⁺	281.0444	281.0444	-0.0	0.00	73.27	13.0

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					

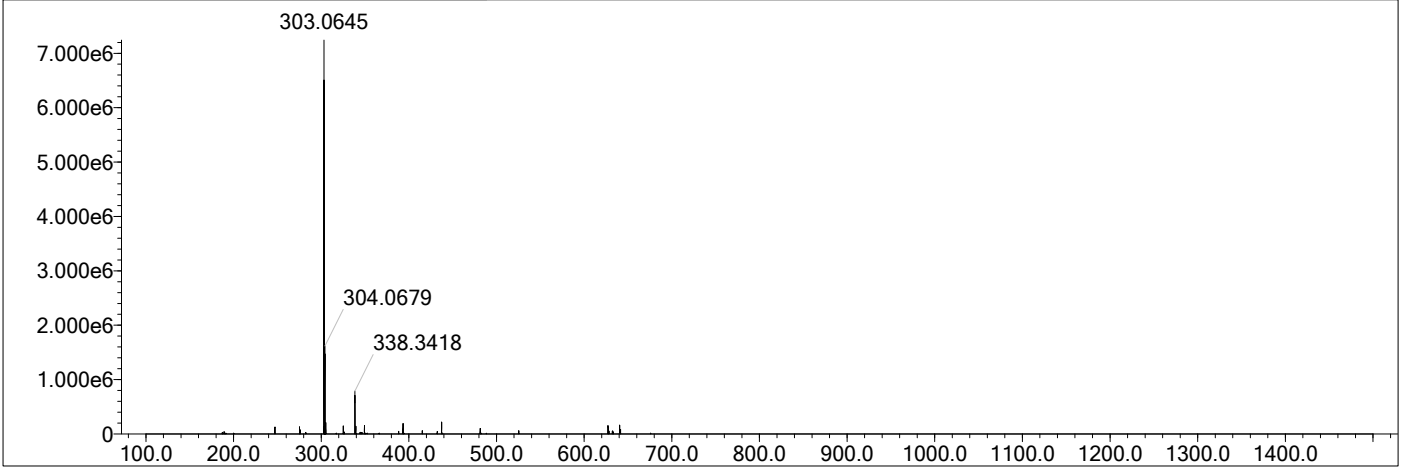
Error Margin (ppm): 100
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

DBE Range: -2.0 - 1000.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

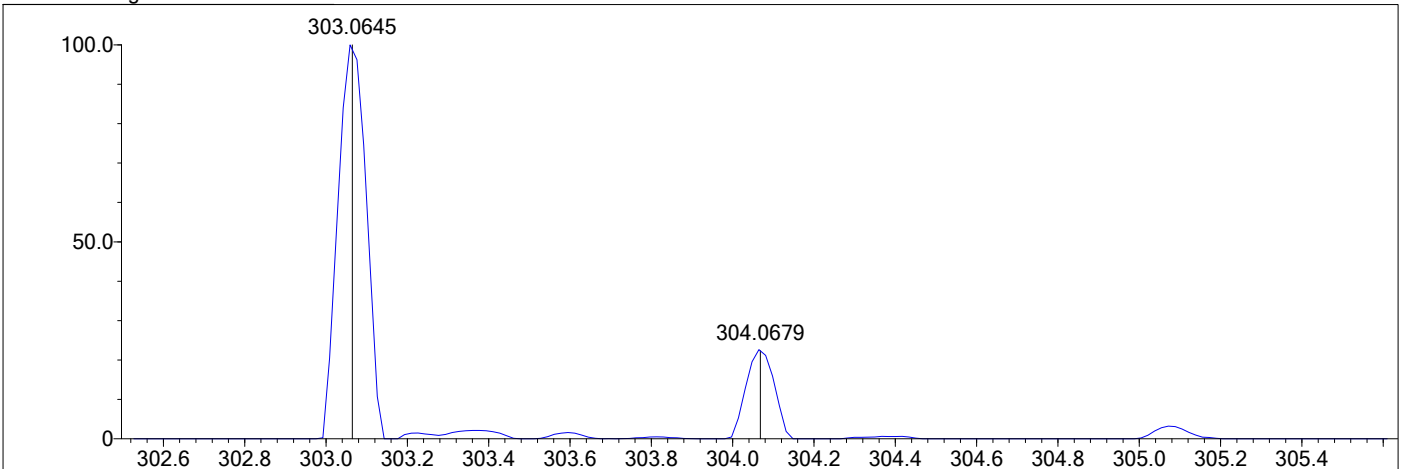
Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

1g

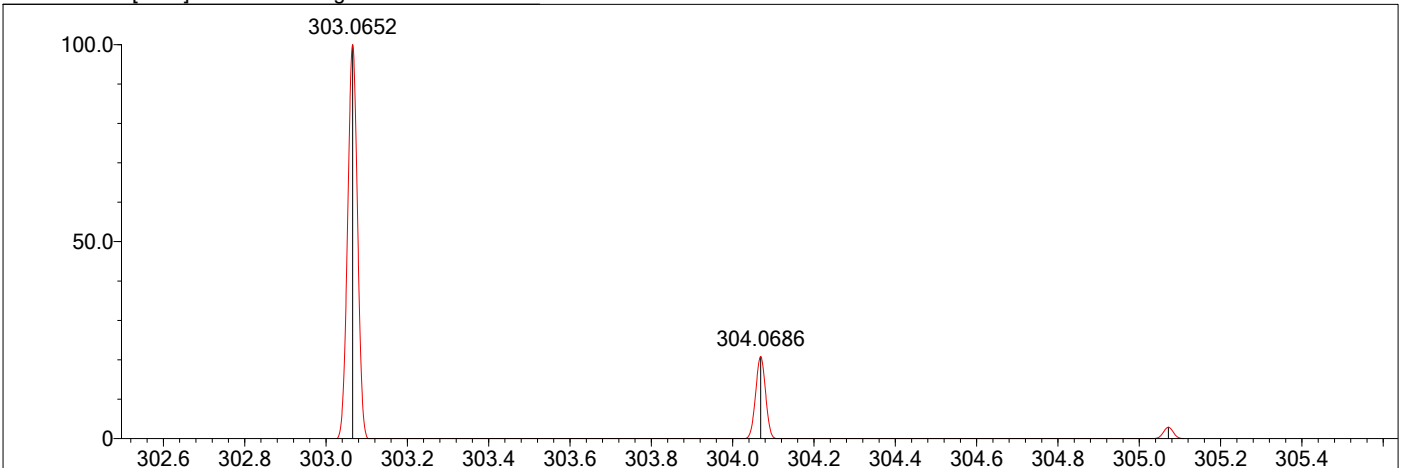
Event#: 1 MS(E+) Ret. Time : 1.120 Scan# : 169



Measured region for 303.0645 m/z



C19 H10 O4 [M+H]⁺ : Predicted region for 303.0652 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	79.30	C19 H10 O4	[M+H] ⁺	303.0645	303.0652	-0.7	-2.31	81.98	15.0

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					

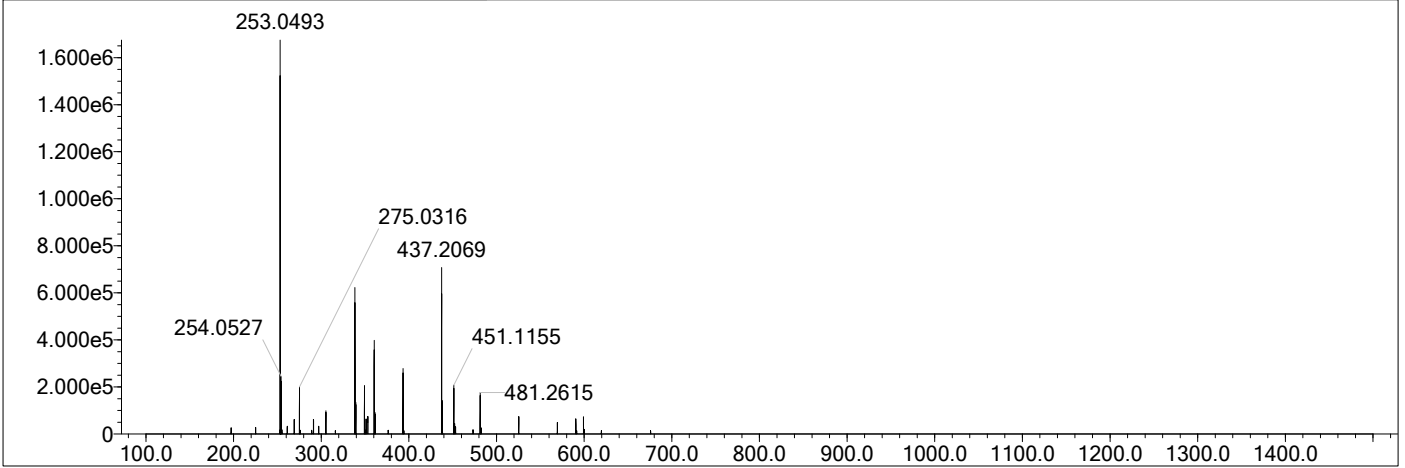
Error Margin (ppm): 100
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

DBE Range: -2.0 - 1000.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

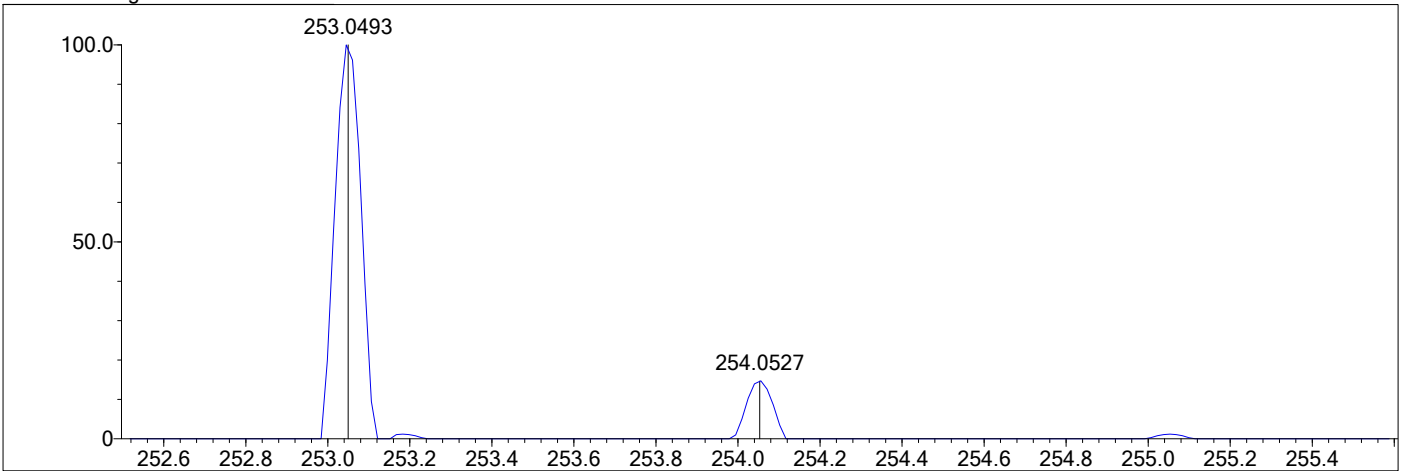
Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

1h

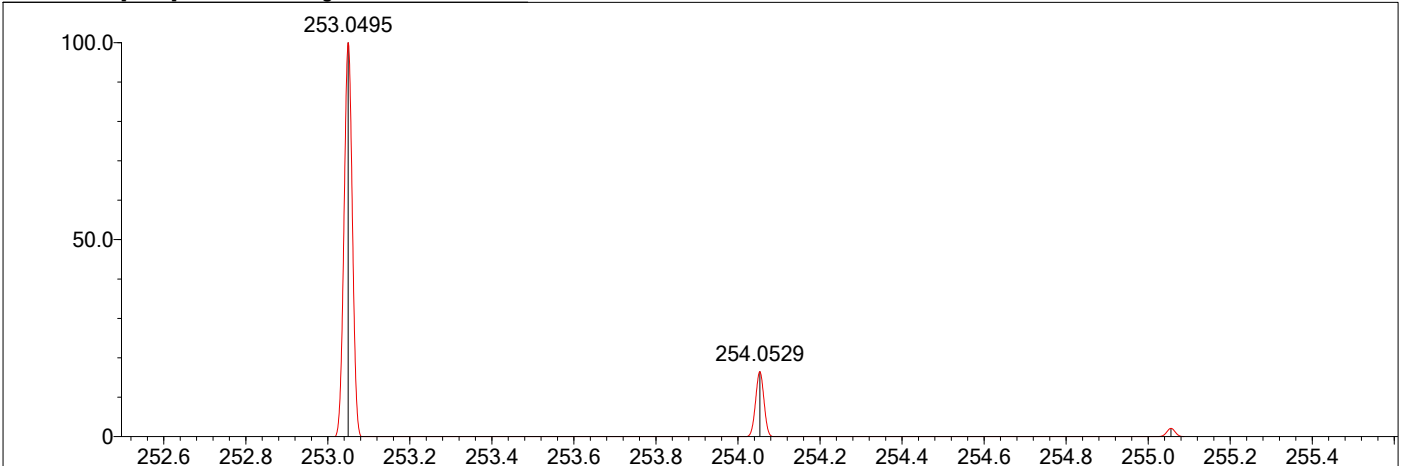
Event#: 1 MS(E+) Ret. Time : 1.213 Scan# : 183



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]+	253.0493	253.0495	-0.2	-0.79	77.50	12.0

Data File: F:\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	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					

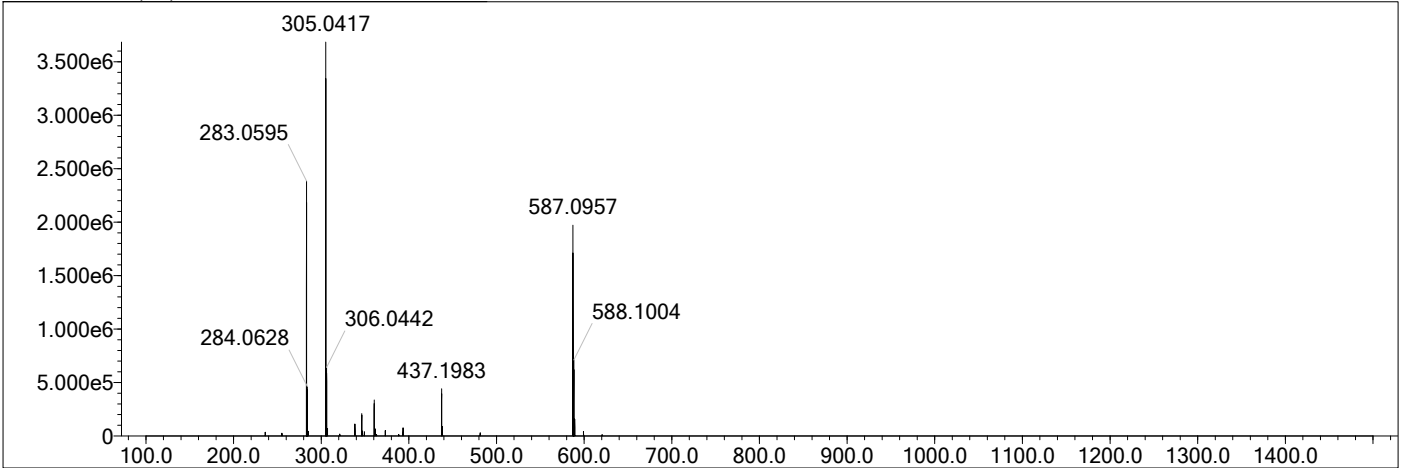
Error Margin (ppm): 100
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

DBE Range: -2.0 - 1000.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

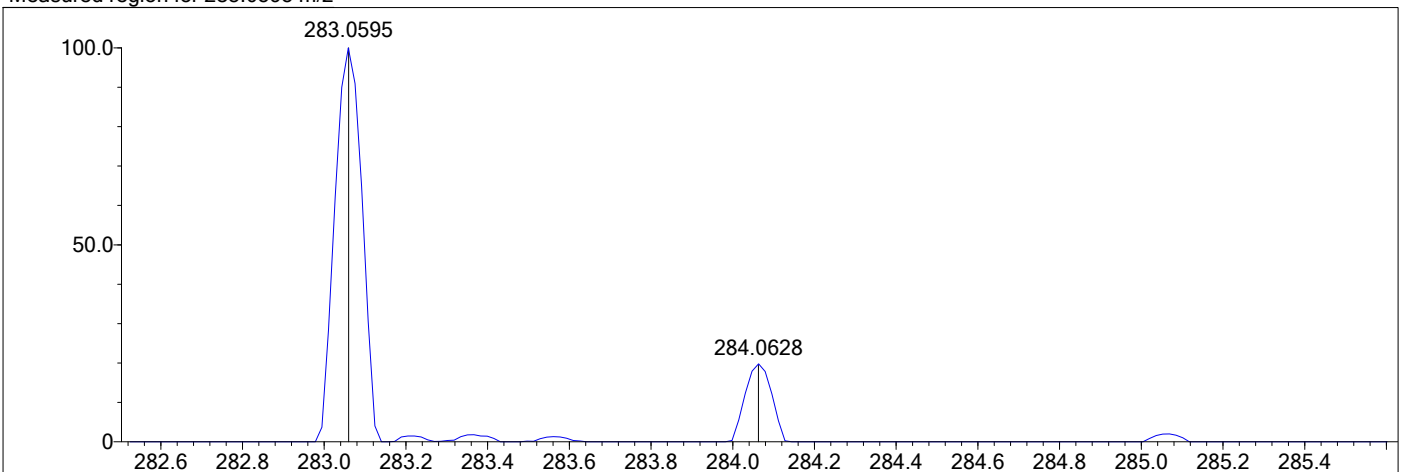
Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

1i

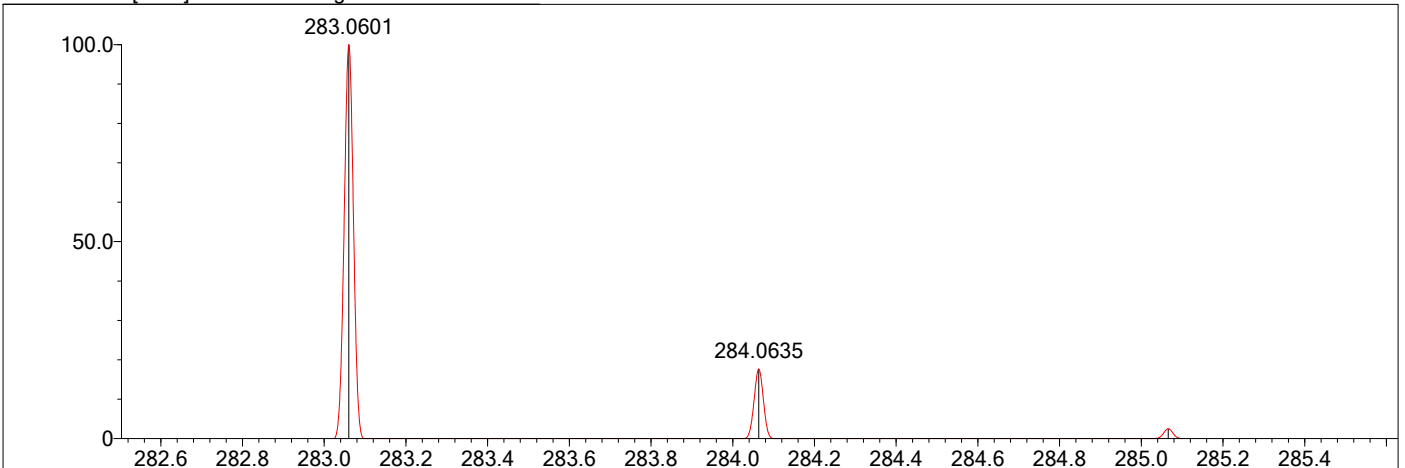
Event#: 1 MS(E+) Ret. Time : 1.227 Scan# : 185



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

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					

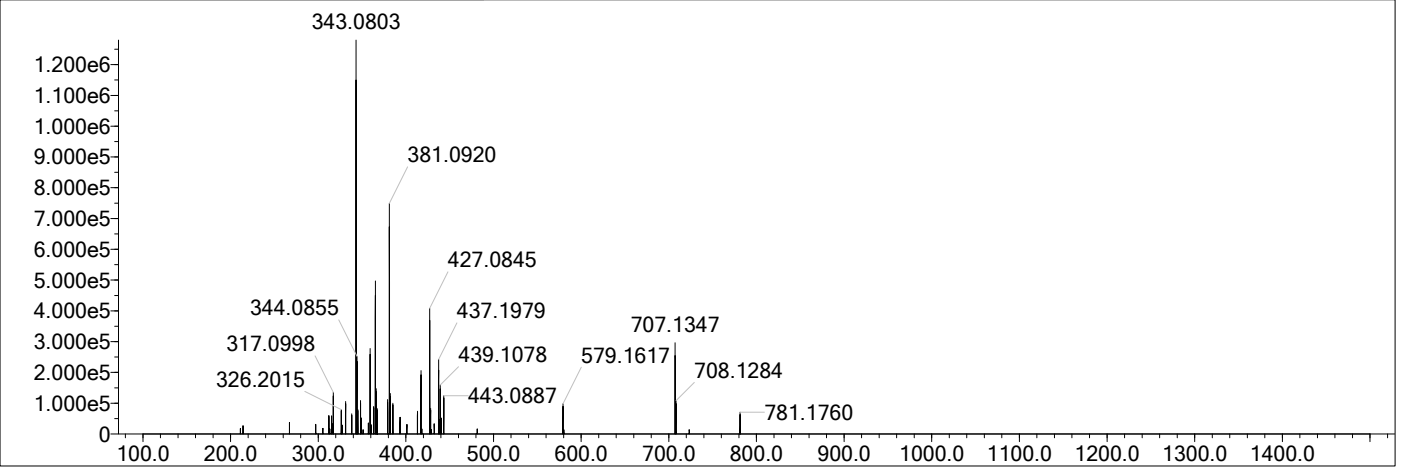
Error Margin (ppm): 100
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

DBE Range: -2.0 - 1000.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

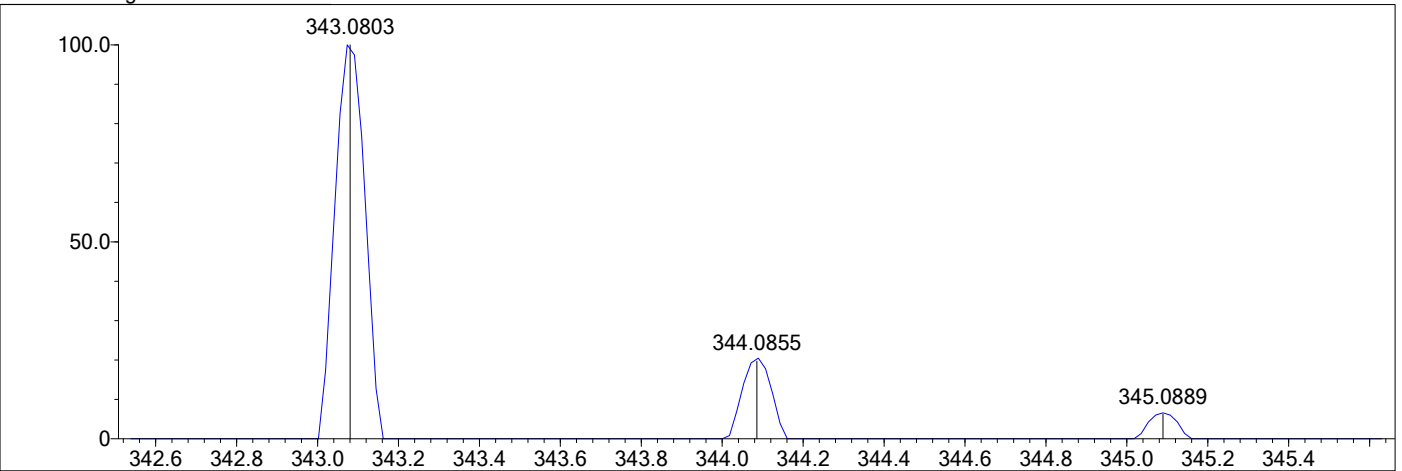
Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

1j

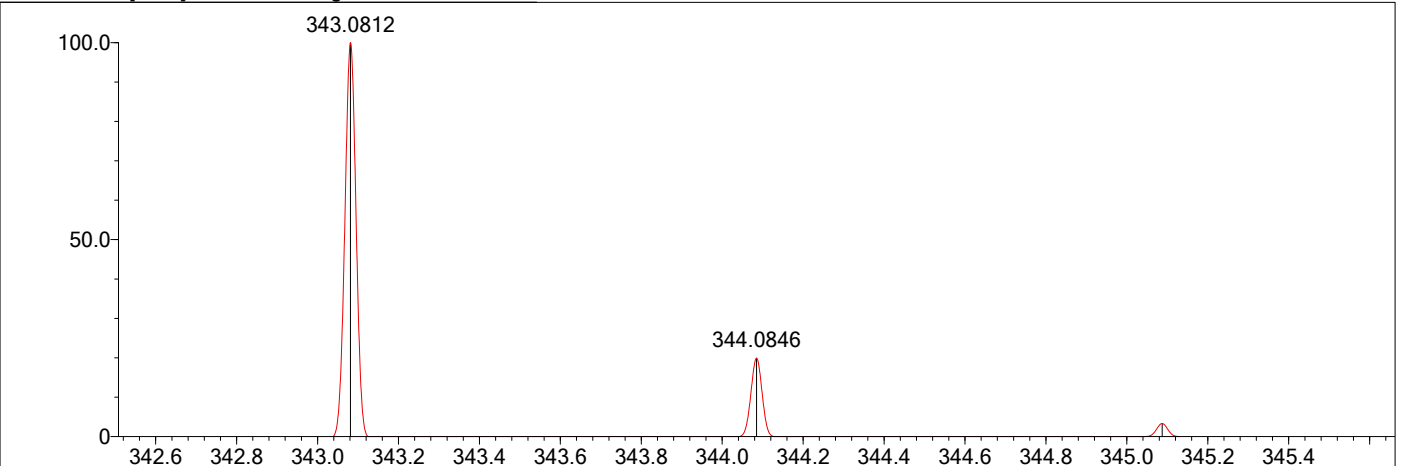
Event#: 1 MS(E+) Ret. Time : 1.133 Scan# : 171



Measured region for 343.0803 m/z



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\邹永\SXH\SJF-1K.Icd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	6	10	O	2	2	3	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	16	S	2	0	0	Se	2	0	0					
N	3	0	0	Cl	1	0	0	Br	1	0	0					

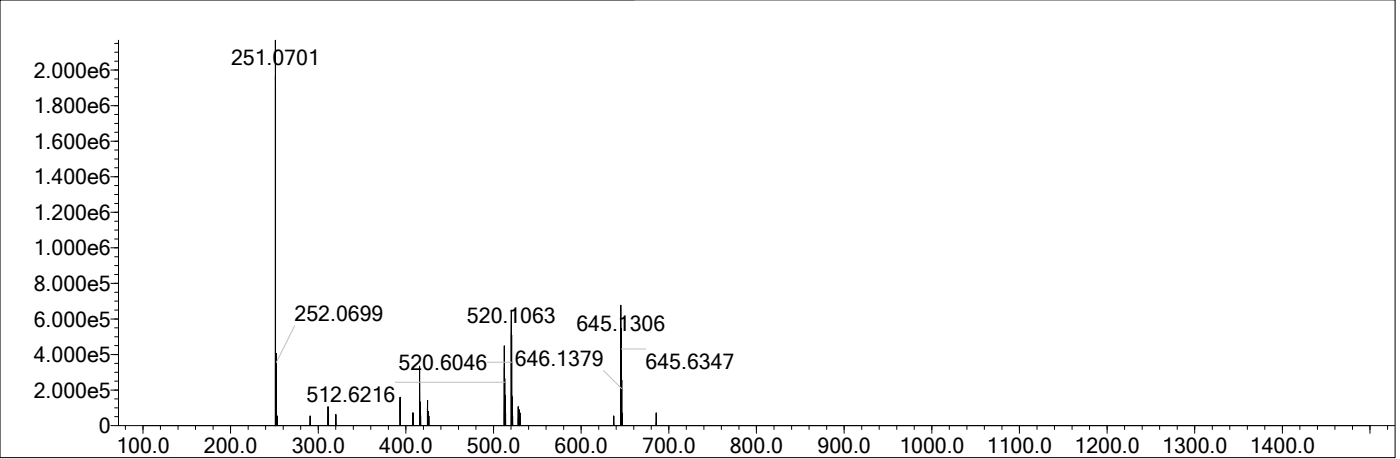
Error Margin (ppm): 100
 HC Ratio: 0.0 - 100.0
 Max Isotopes: all
 MSn Iso RI (%): 75.00

DBE Range: -100.0 - 200.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

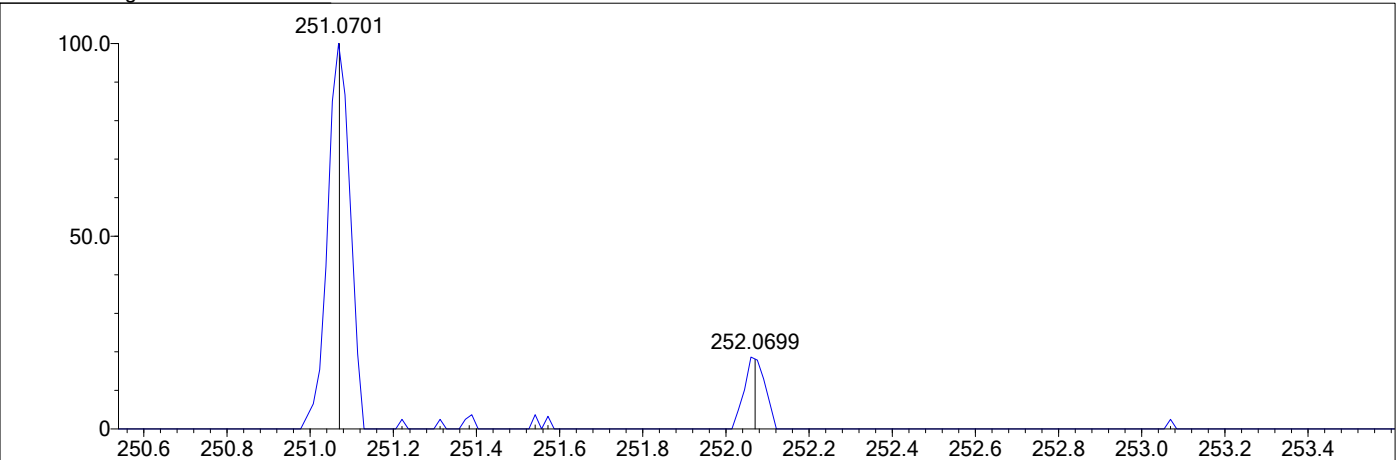
Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 100

1k

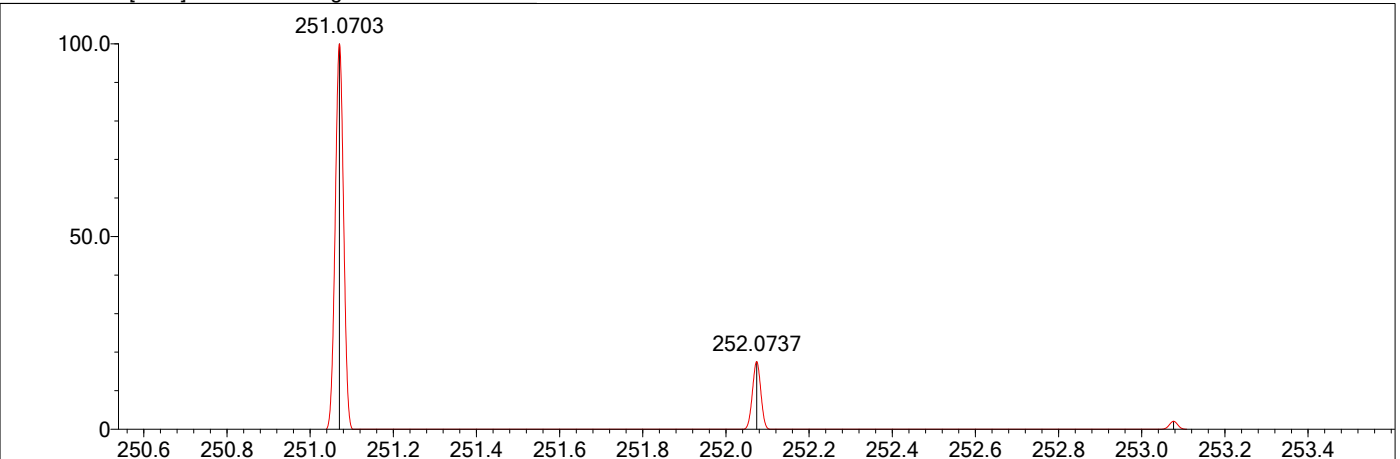
Event#: 1 MS(E+) Ret. Time : 1.320 -> 1.320 Scan# : 199 -> 199



Measured region for 251.0701 m/z



C16 H10 O3 [M+H]+ : Predicted region for 251.0703 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	69.28	C16 H10 O3	[M+H]+	251.0701	251.0703	-0.2	-0.80	69.28	12.0

Data File: F:\高分辨数据\Zouyong\sjf\S10.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					

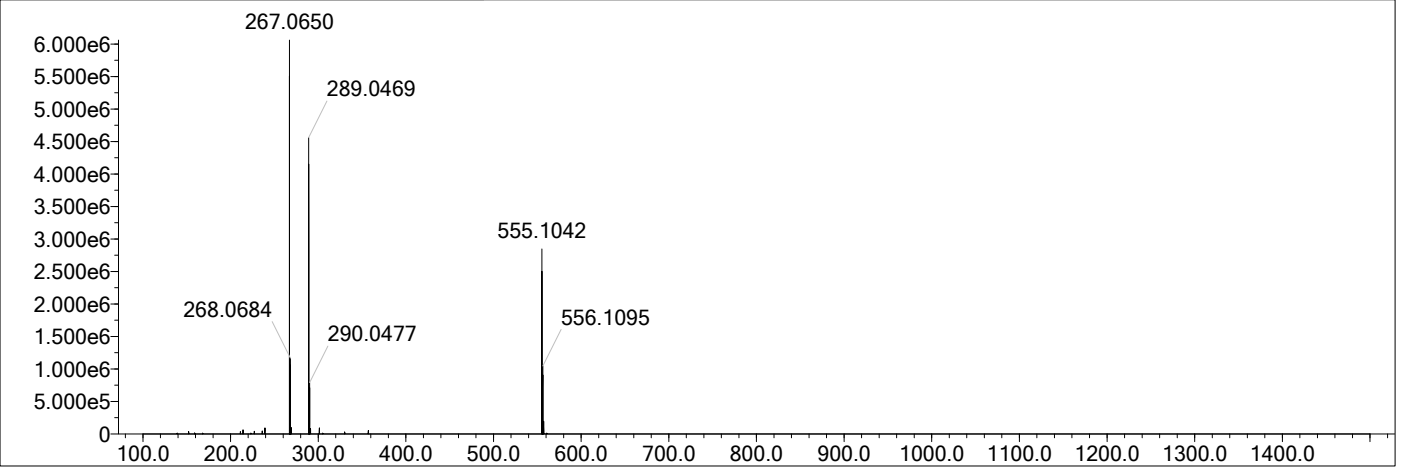
Error Margin (ppm): 100
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

DBE Range: -2.0 - 1000.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

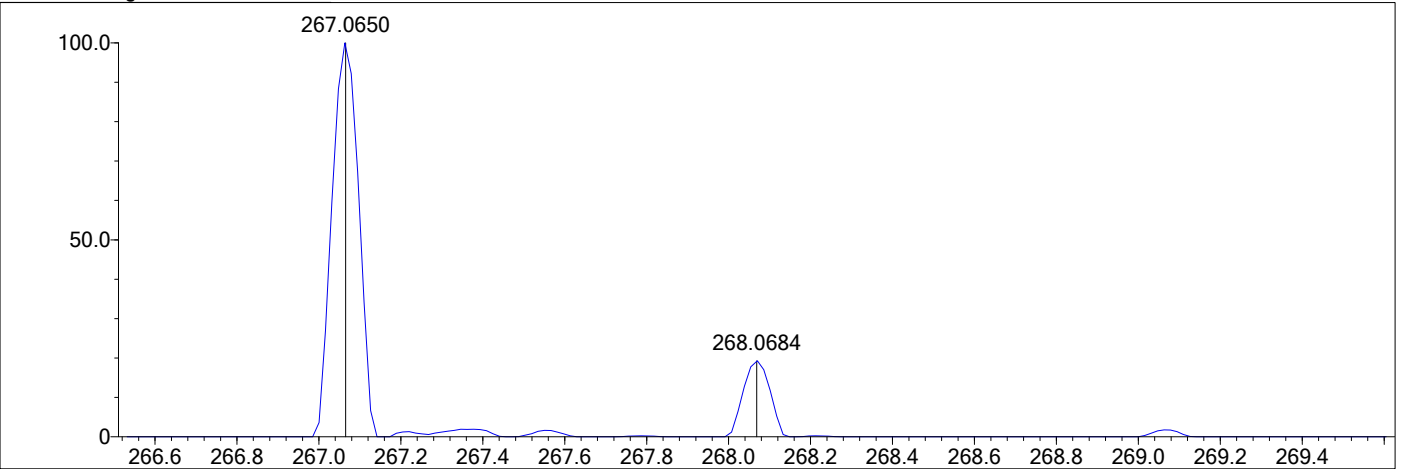
Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

11

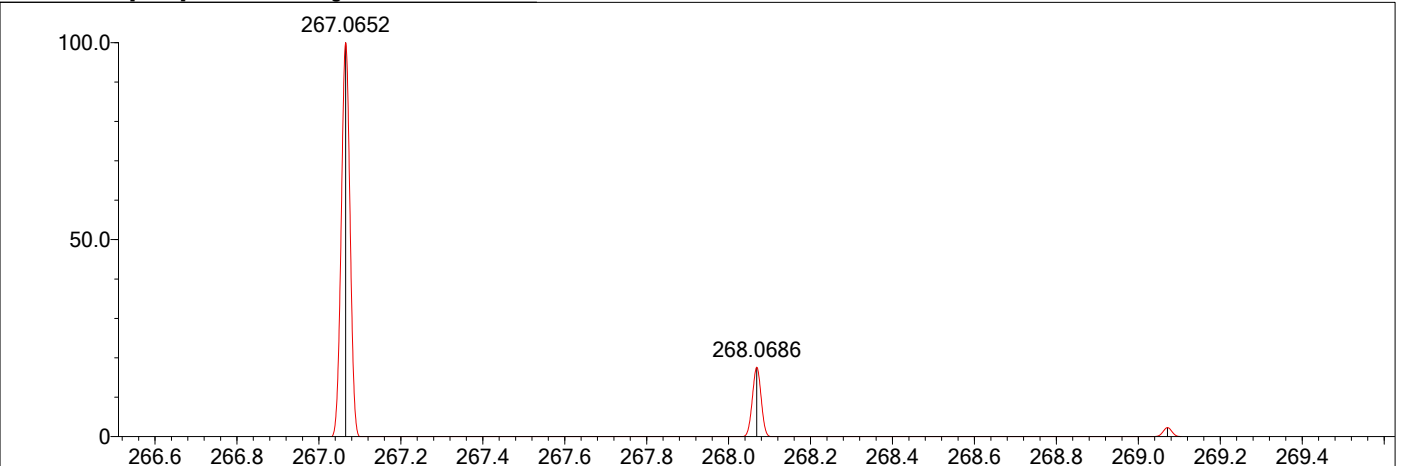
Event#: 1 MS(E+) Ret. Time : 1.560 Scan# : 235



Measured region for 267.0650 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	73.11	C16 H10 O4	[M+H] ⁺	267.0650	267.0652	-0.2	-0.75	73.11	12.0

Data File: F:\高分辨数据\Zouyong\sjf\S15.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	1	1	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					

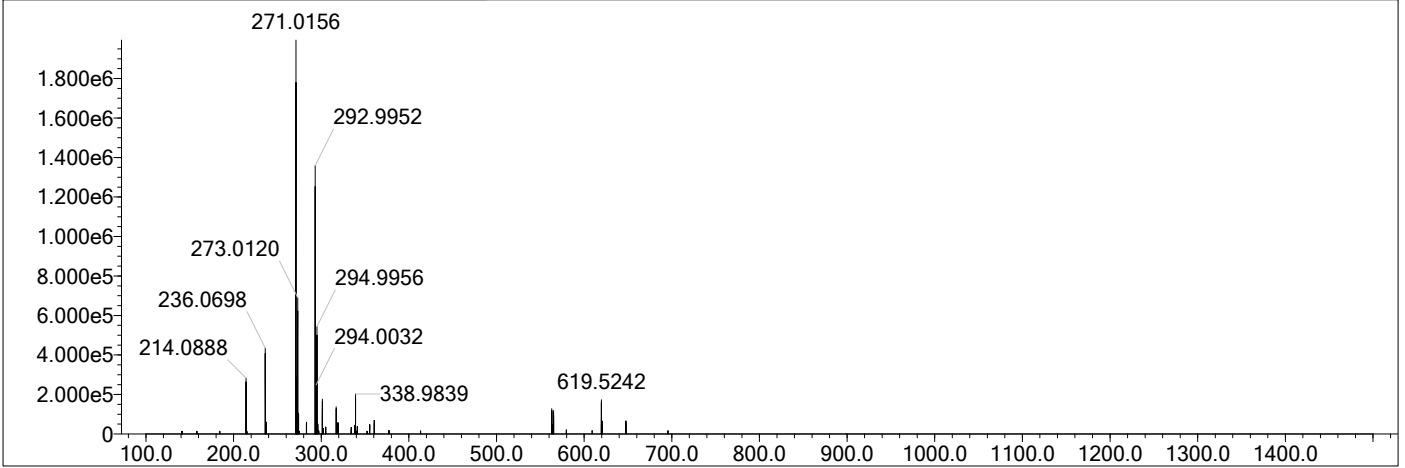
Error Margin (ppm): 100
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

DBE Range: -2.0 - 1000.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

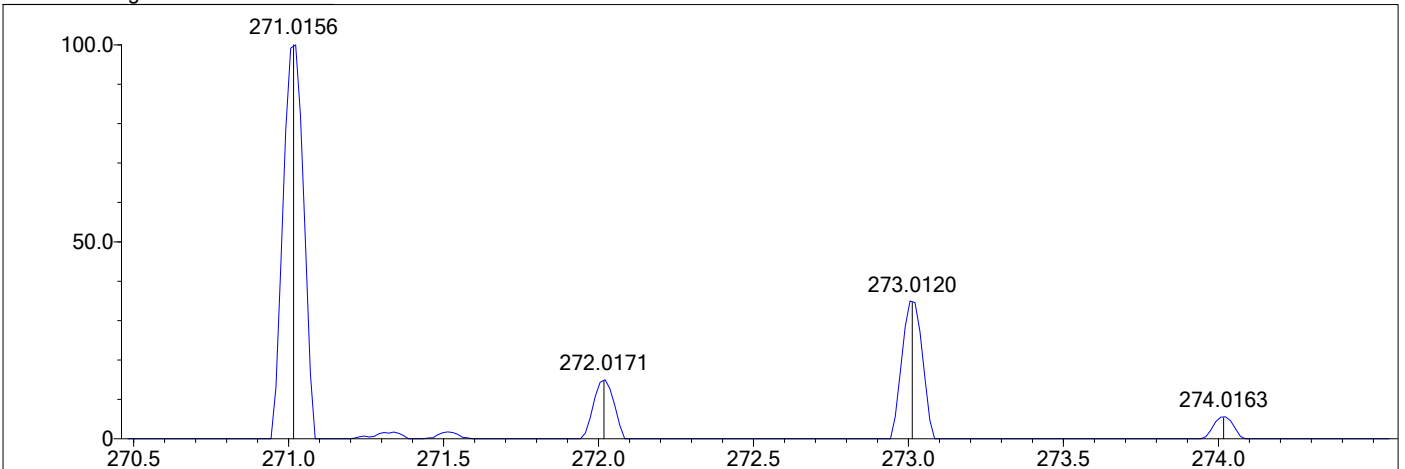
Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

1m

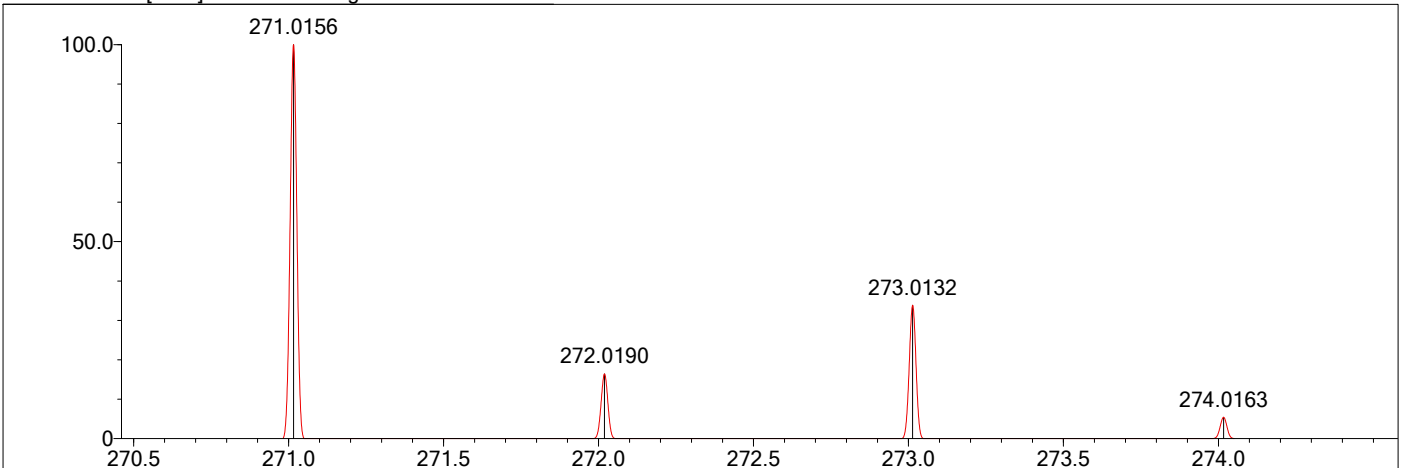
Event#: 1 MS(E+) Ret. Time : 1.680 Scan# : 253



Measured region for 271.0156 m/z



C15 H7 O3 Cl [M+H]+ : Predicted region for 271.0156 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	78.35	C15 H7 O3 Cl	[M+H]+	271.0156	271.0156	-0.0	0.00	78.35	12.0

Data File: F:\高分辨数据\Zouyong\sjf\S11.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					

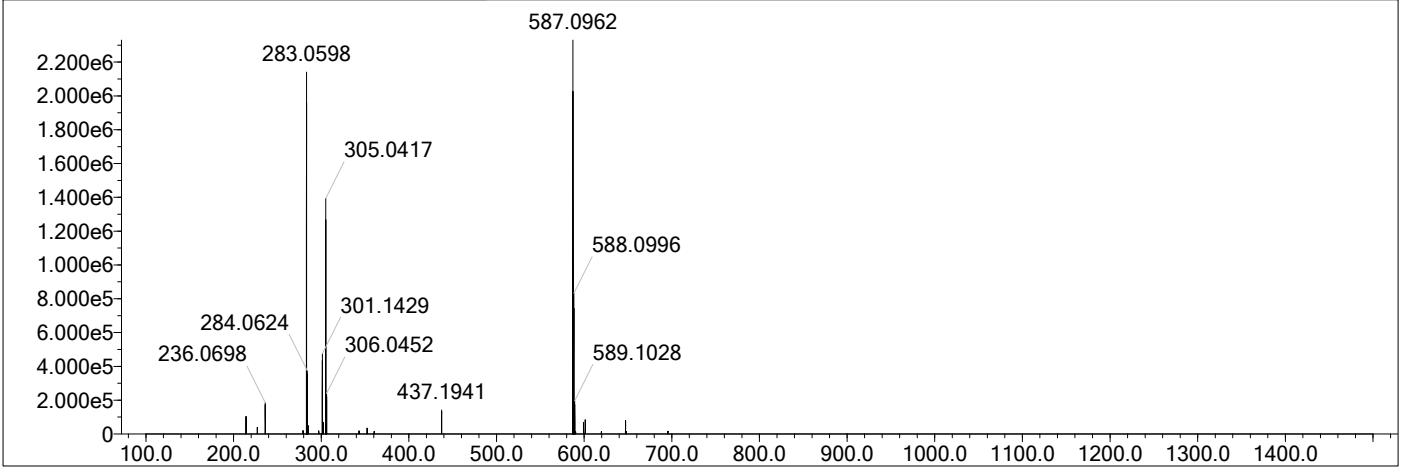
Error Margin (ppm): 100
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

DBE Range: -2.0 - 1000.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

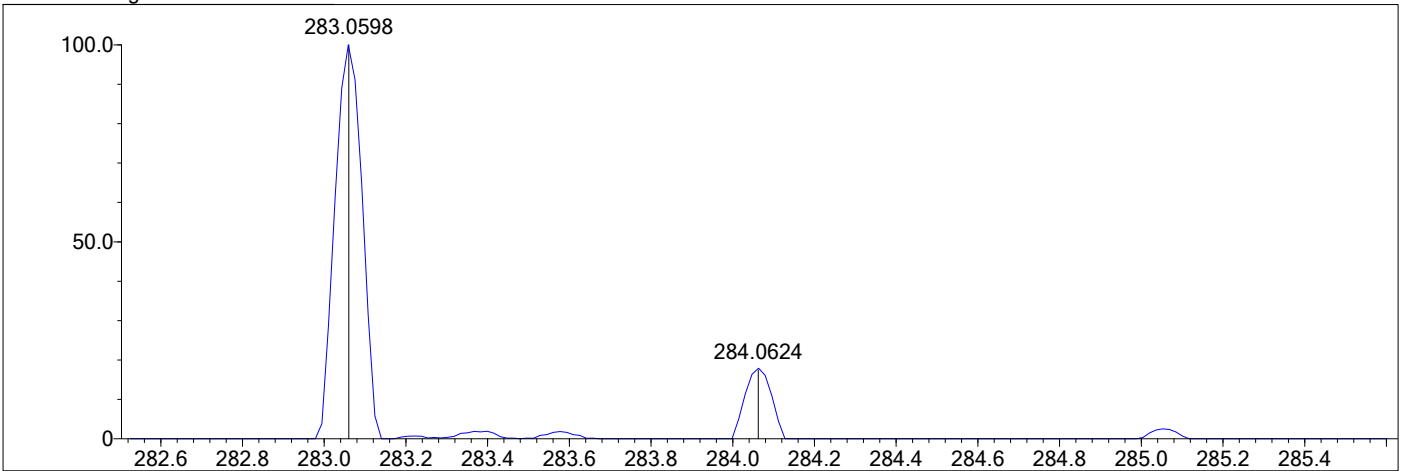
Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

1n

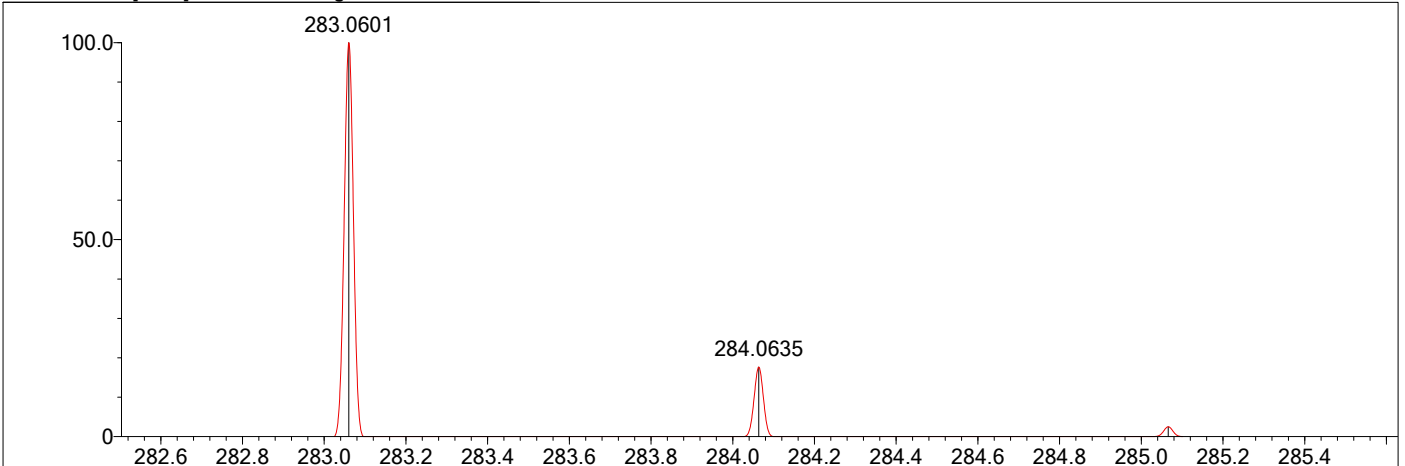
Event#: 1 MS(E+) Ret. Time : 1.360 Scan# : 205



Measured region for 283.0598 m/z



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



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	76.34	C16 H10 O5	[M+H]+	283.0598	283.0601	-0.3	-1.06	76.45	12.0

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	
C	4	0	60	Na	1	0	0	K	1	0	0					
N	3	0	0	Si	4	0	0	Mn	3	0	0					

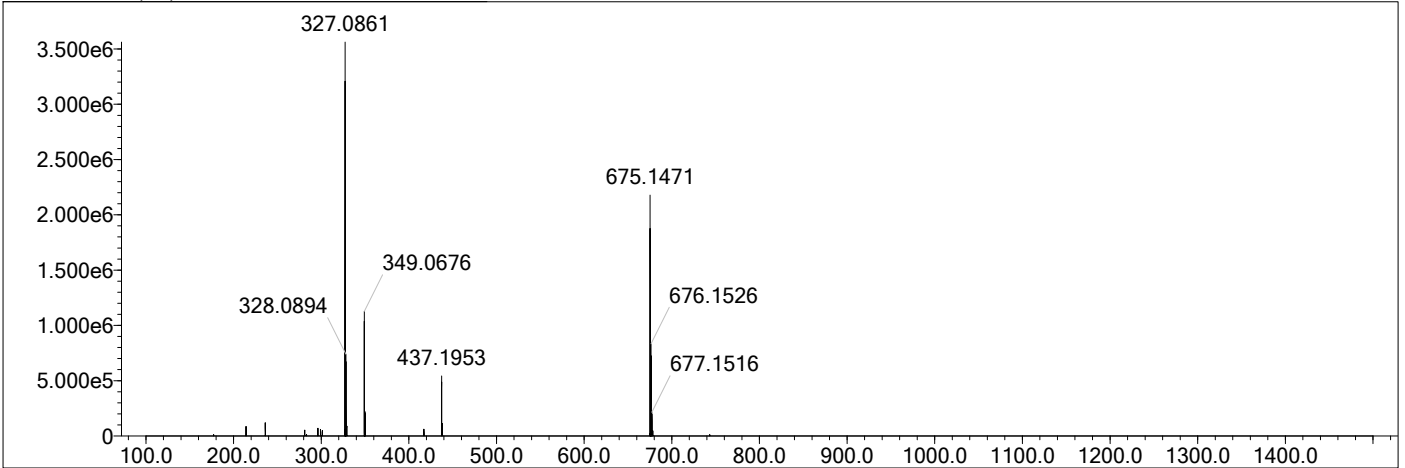
Error Margin (ppm): 100
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

DBE Range: -2.0 - 1000.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

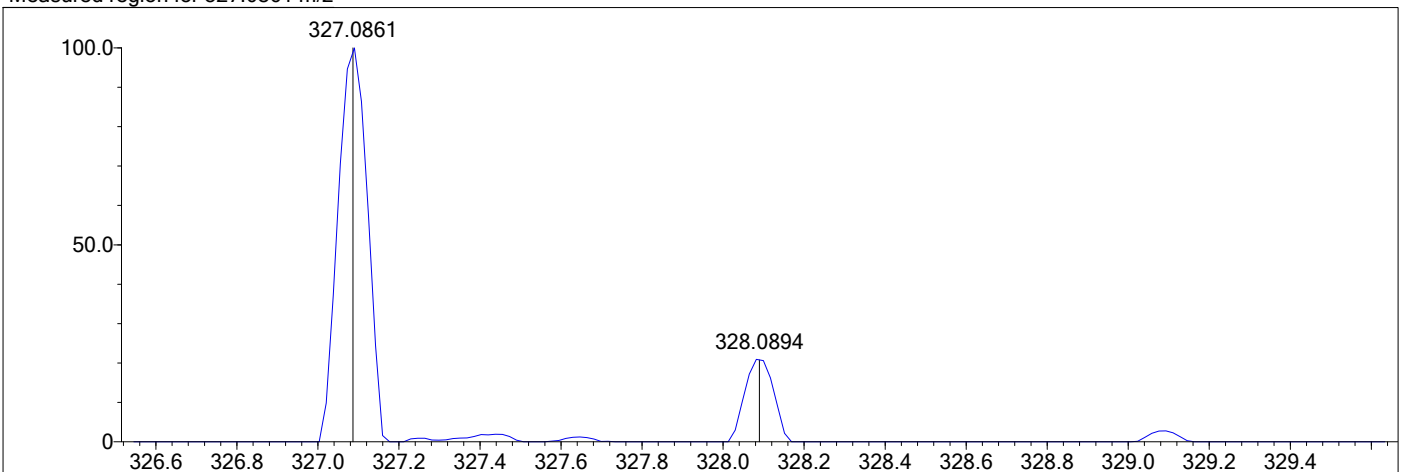
Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

10

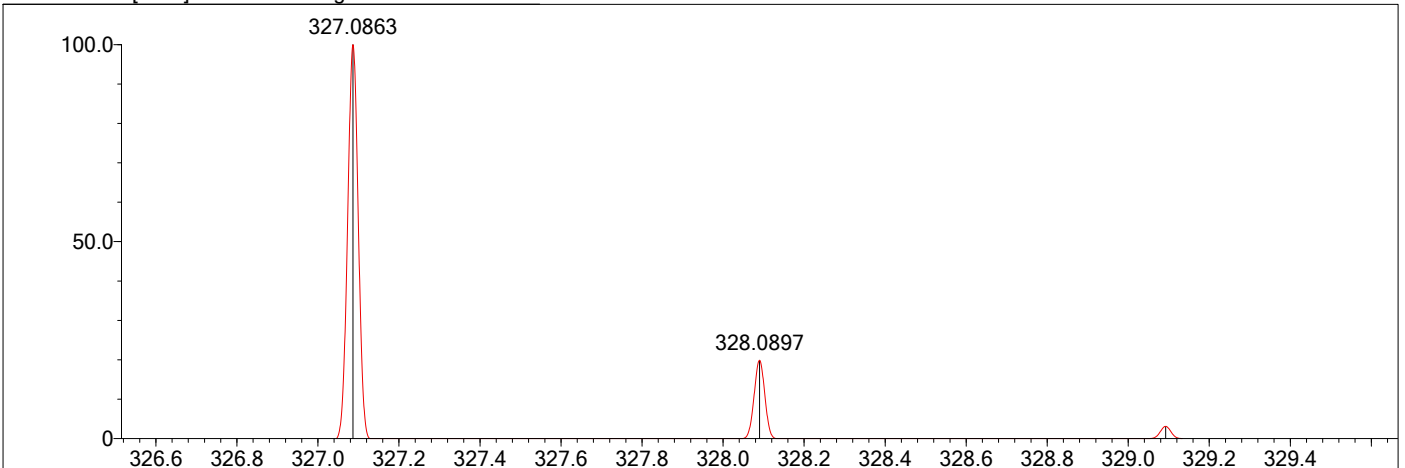
Event#: 1 MS(E+) Ret. Time : 1.280 Scan# : 193



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: F:\高分辨数据\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					

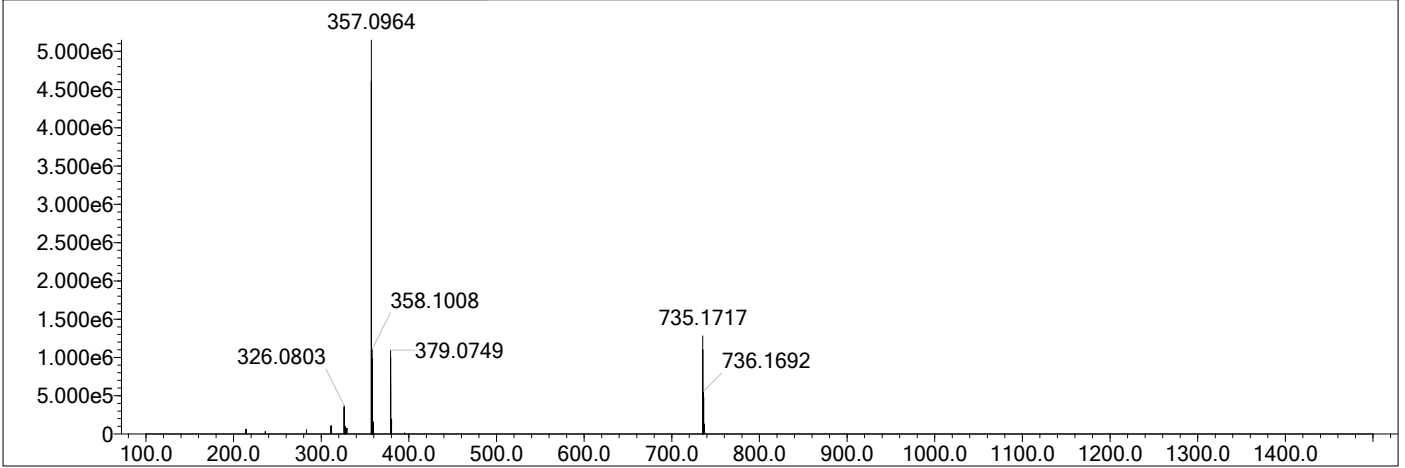
Error Margin (ppm): 100
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

DBE Range: -2.0 - 1000.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

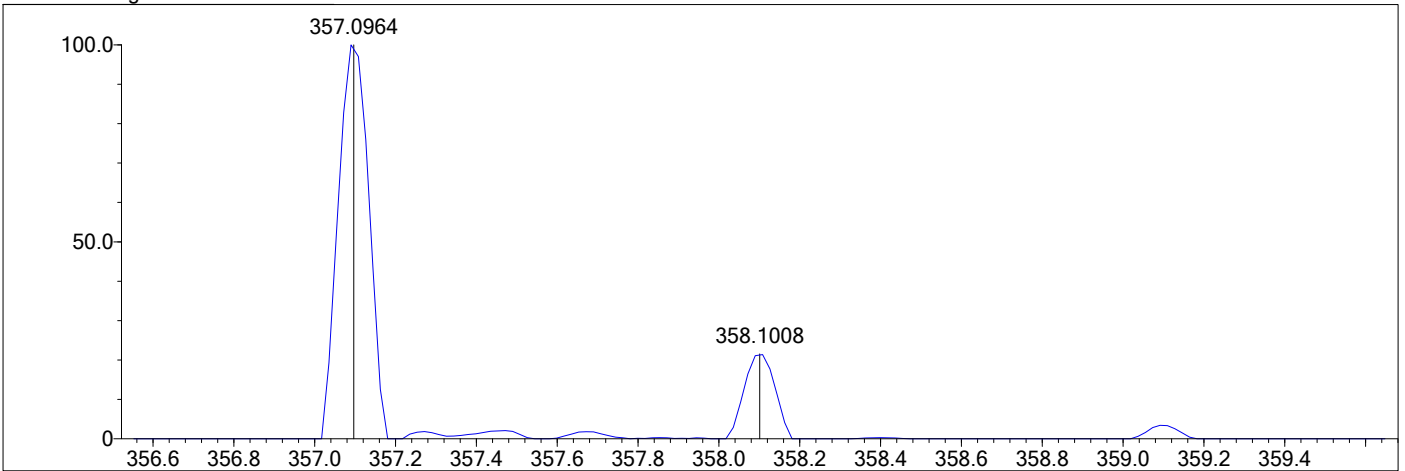
Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

1p

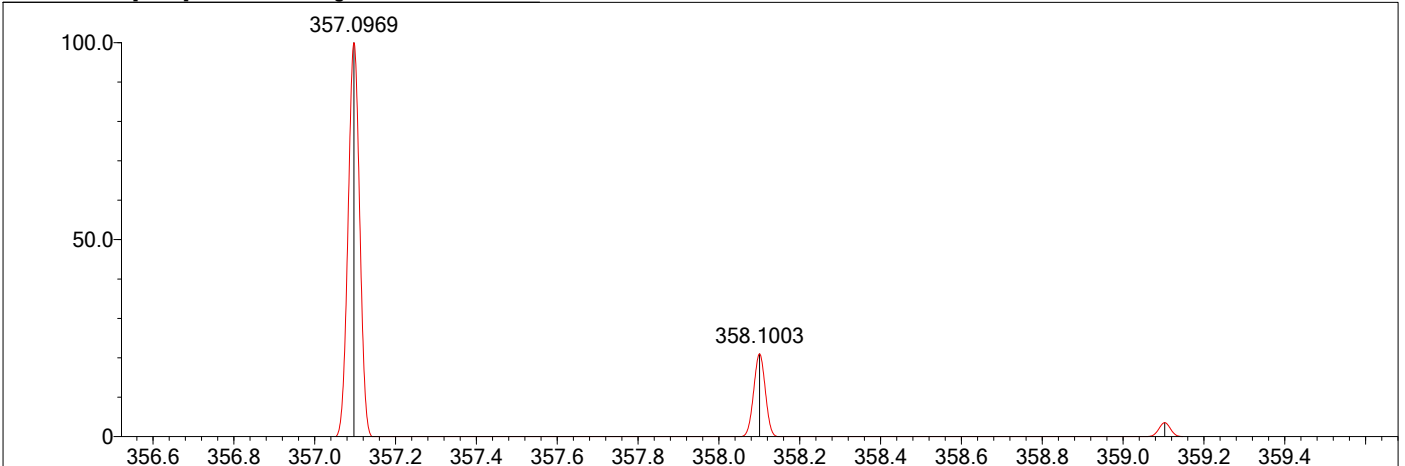
Event#: 1 MS(E+) Ret. Time : 1.307 Scan# : 197



Measured region for 357.0964 m/z



C19H16O7 [M+H]⁺ : Predicted region for 357.0969 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	82.79	C19H16O7	[M+H] ⁺	357.0964	357.0969	-0.5	-1.40	83.63	12.0

Data File: F:\高分辨数据\Zouyong\sjf\S14.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					

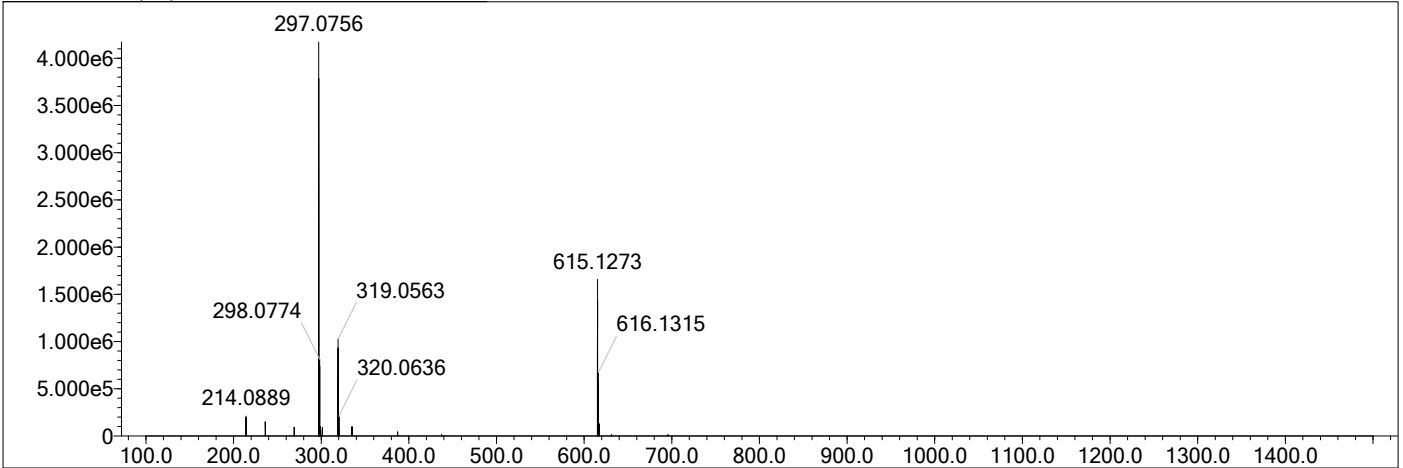
Error Margin (ppm): 100
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

DBE Range: -2.0 - 1000.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

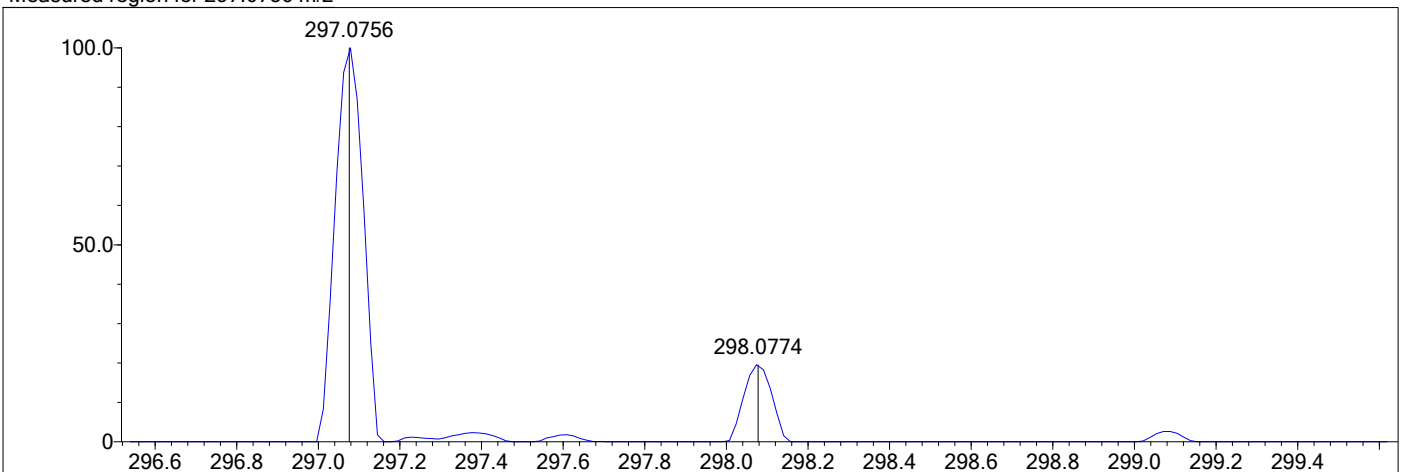
Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

1q

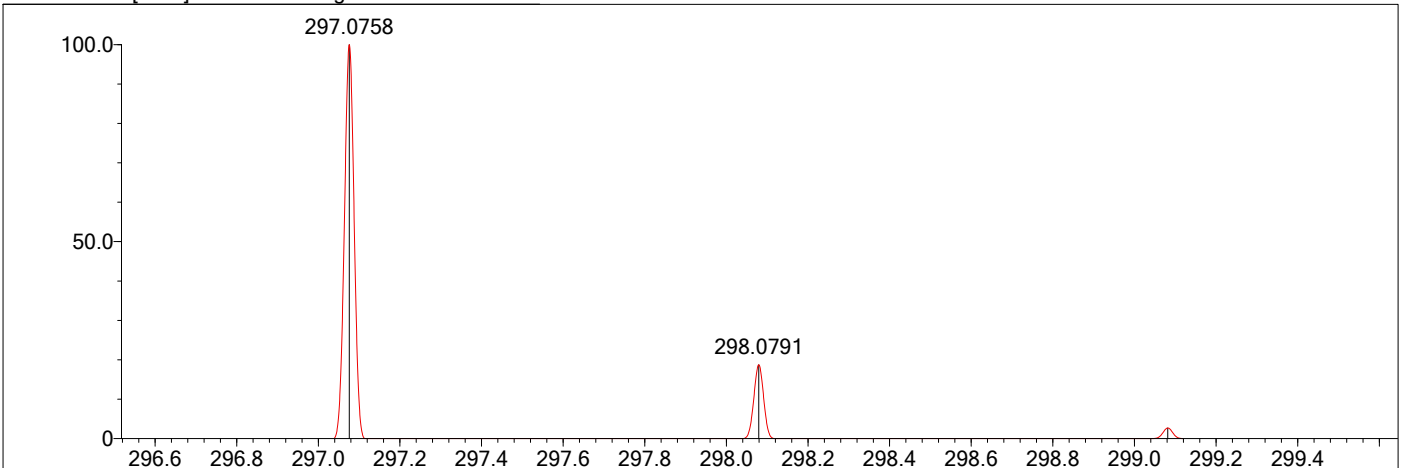
Event#: 1 MS(E+) Ret. Time : 1.693 Scan# : 255



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-20160624\data1\邹永\SXH\SJF-1R.lcd

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
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	18	19	S	2	0	0	Se	2	0	0					
N	3	0	0	Cl	1	0	0	Br	1	0	0					

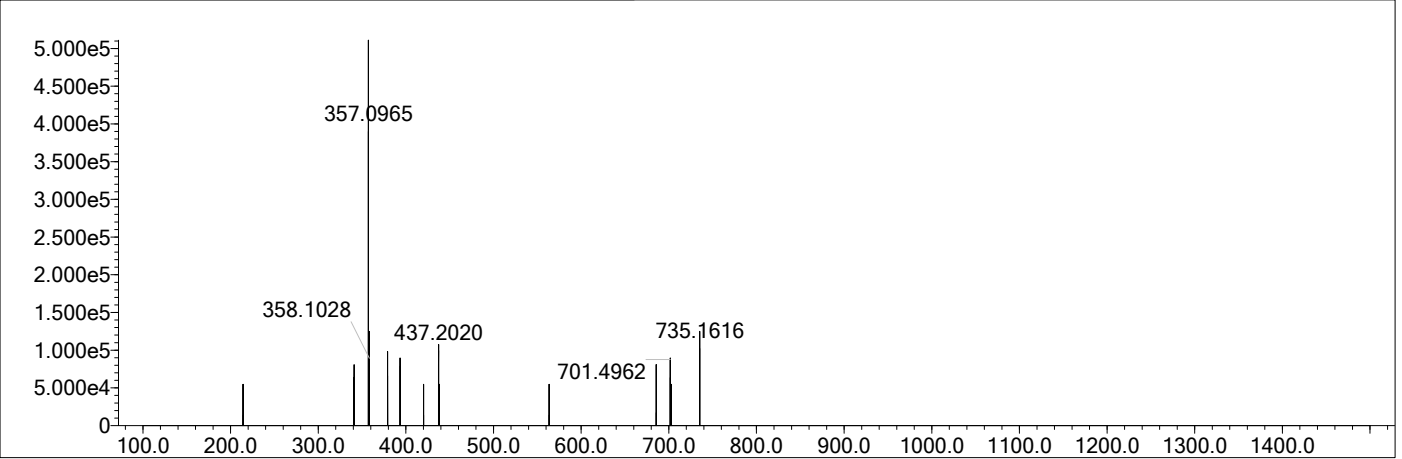
Error Margin (ppm): 100
 HC Ratio: 0.0 - 100.0
 Max Isotopes: all
 MSn Iso RI (%): 75.00

DBE Range: -100.0 - 200.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

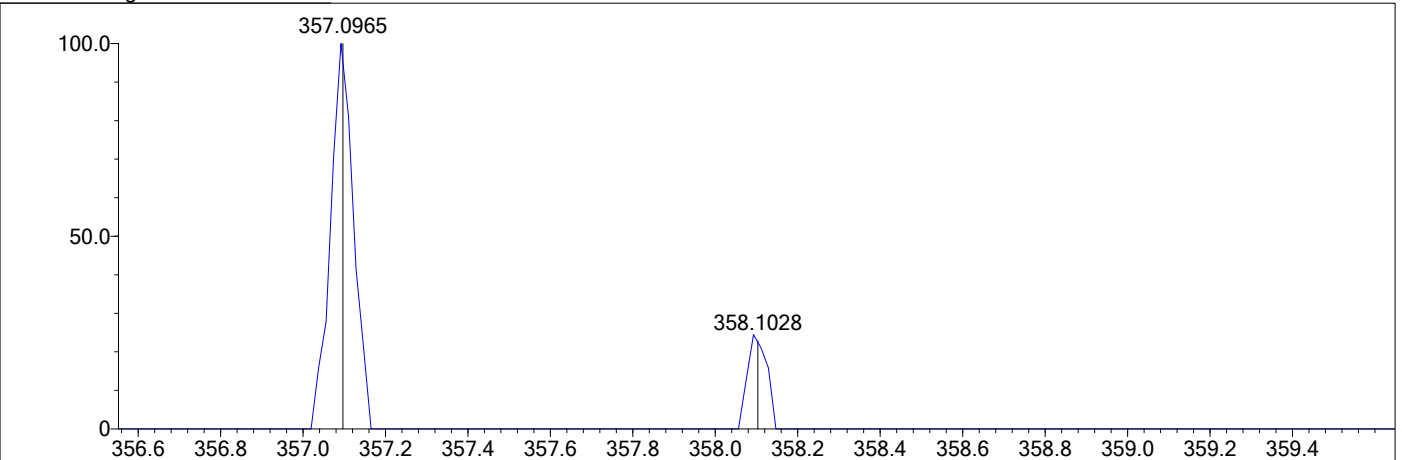
Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 100

1r

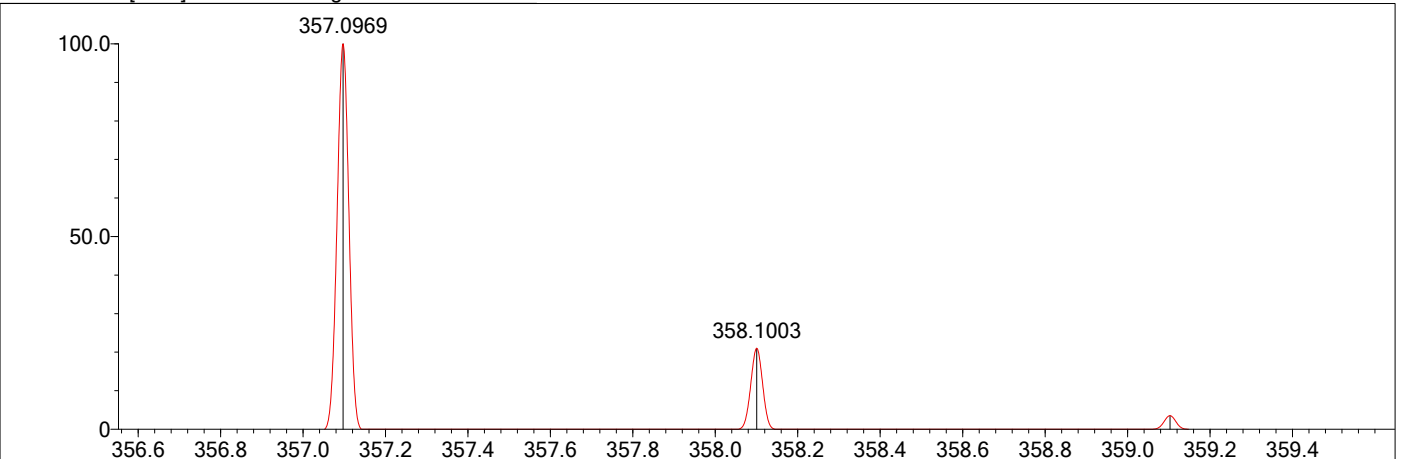
Event#: 1 MS(E+) Ret. Time : 1.040 -> 1.040 Scan# : 157 -> 157



Measured region for 357.0965 m/z



C19 H16 O7 [M+H]⁺ : Predicted region for 357.0969 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	72.56	C19 H16 O7	[M+H] ⁺	357.0965	357.0969	-0.4	-1.12	72.78	12.0

Data File: \\Deep-20160624\data1\邹永\SXH\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	S	2	0	0	Se	2	0	0					
N	3	0	0	Cl	1	0	0	Br	1	0	0					

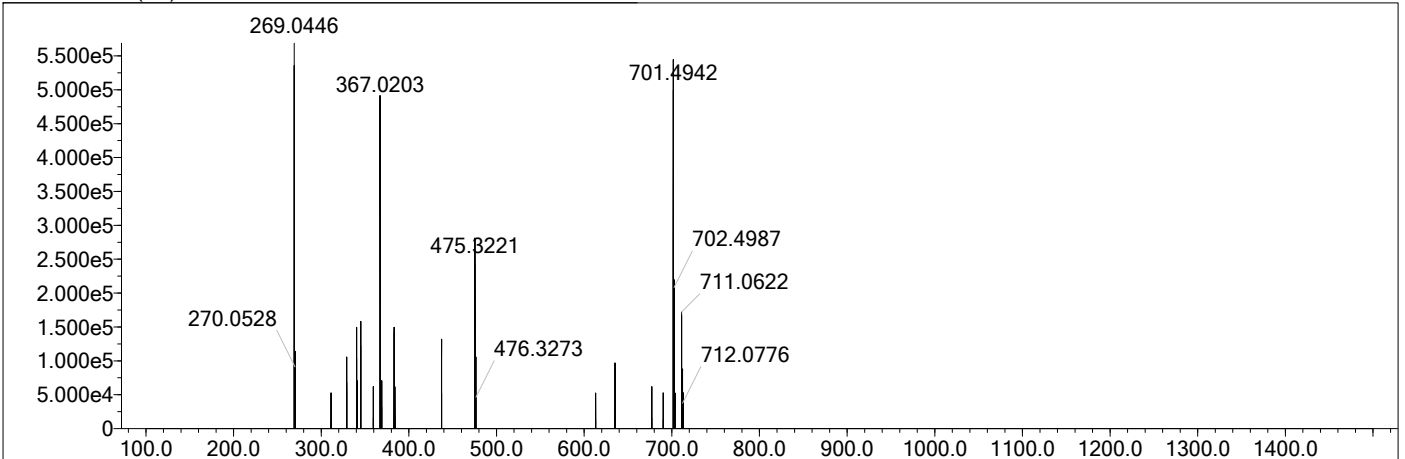
Error Margin (ppm): 100
 HC Ratio: 0.0 - 100.0
 Max Isotopes: all
 MSn Iso RI (%): 75.00

DBE Range: -100.0 - 200.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

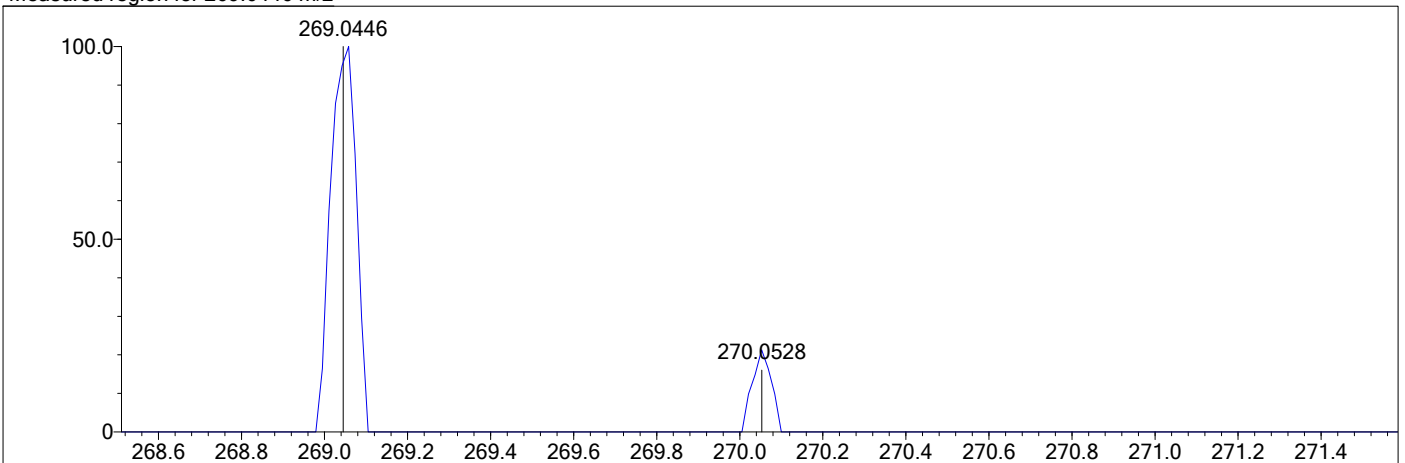
Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 100

1s

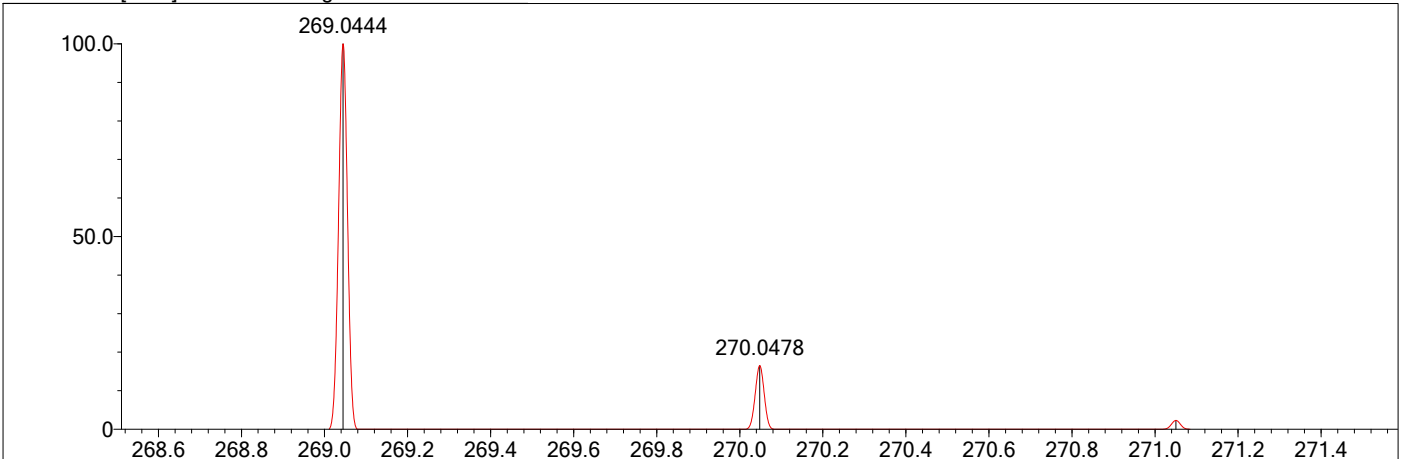
Event#: 1 MS(E+) Ret. Time: 0.800 -> 0.800 Scan#: 121 -> 121



Measured region for 269.0446 m/z



C15 H8 O5 [M+H]+ : Predicted region for 269.0444 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	62.11	C15 H8 O5	[M+H]+	269.0446	269.0444	0.2	0.74	62.11	12.0

Data File: F:\高分辨数据\Zouyong\sjf\S16.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					

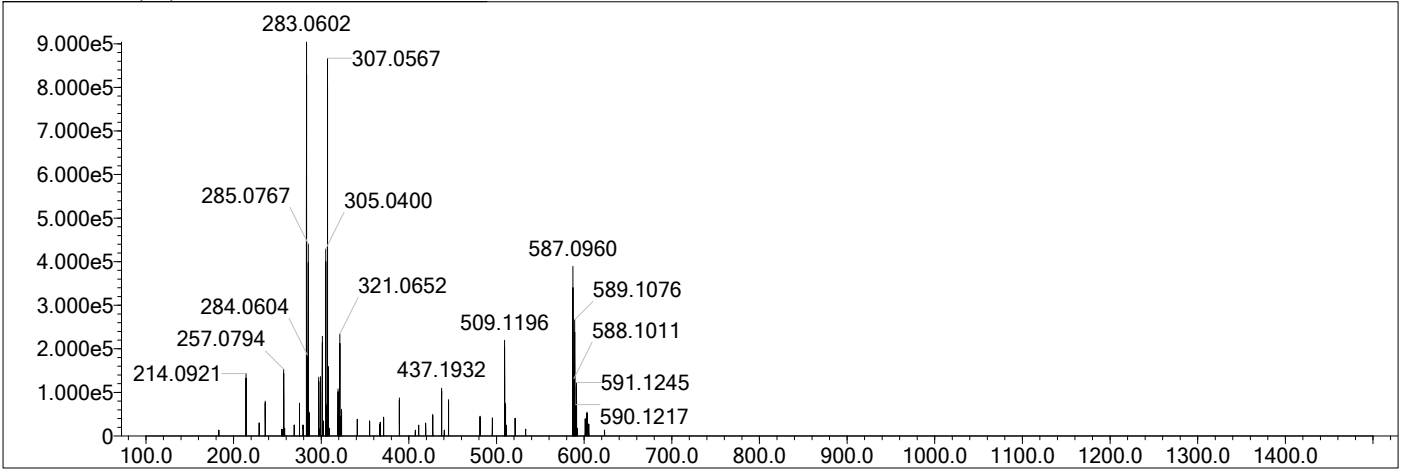
Error Margin (ppm): 100
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

DBE Range: -2.0 - 1000.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

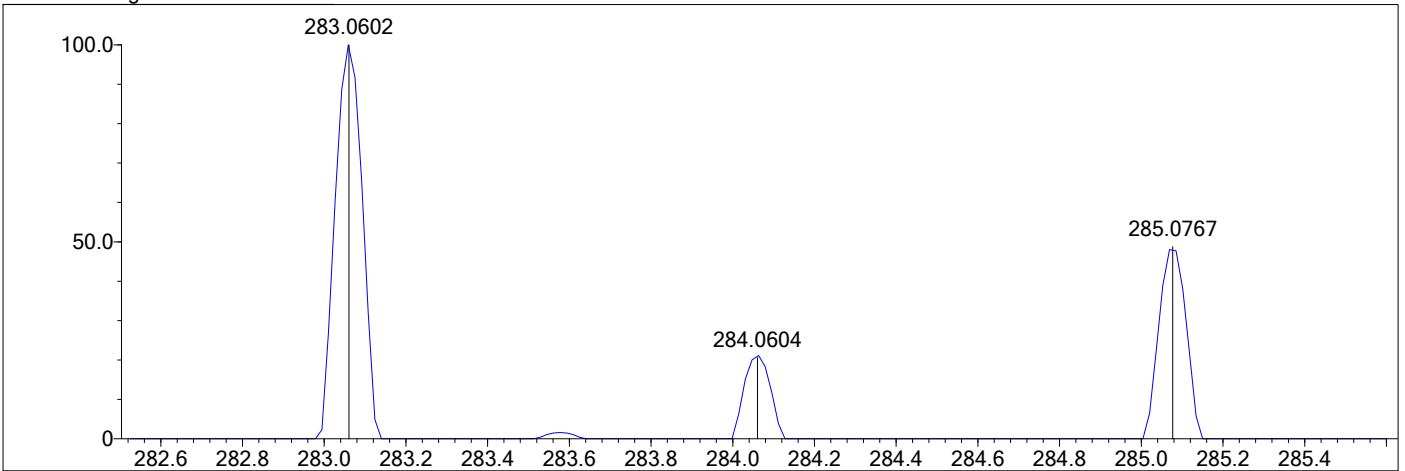
Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

1t

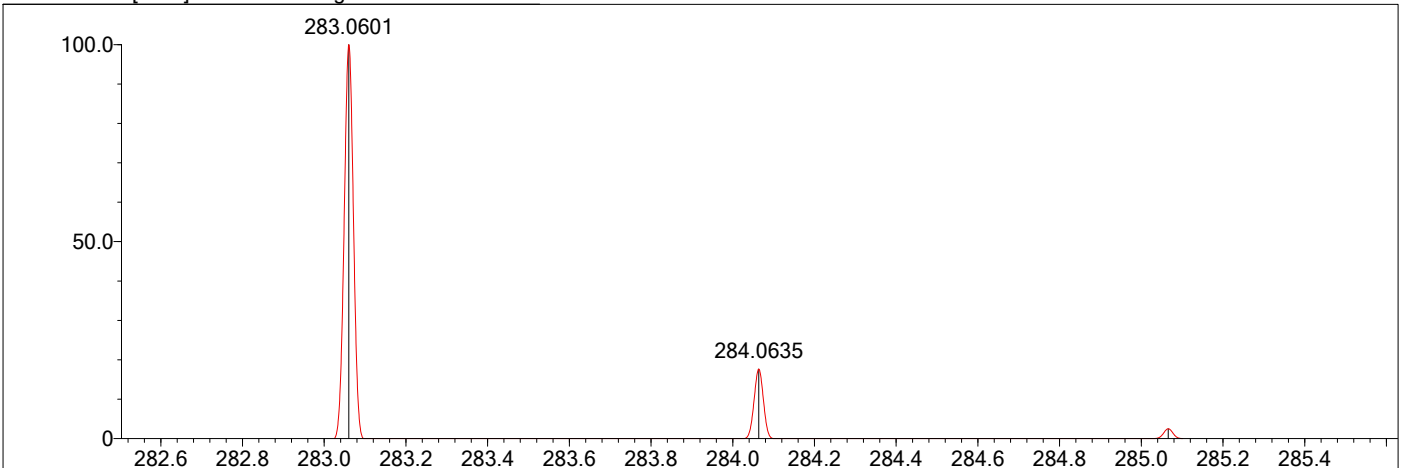
Event#: 1 MS(E+) Ret. Time : 1.333 Scan# : 201



Measured region for 283.0602 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	29.38	C16 H10 O5	[M+H] ⁺	283.0602	283.0601	0.1	0.35	29.38	12.0

Data File: F:\高分辨数据\Zouyong\sjf\S17.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					

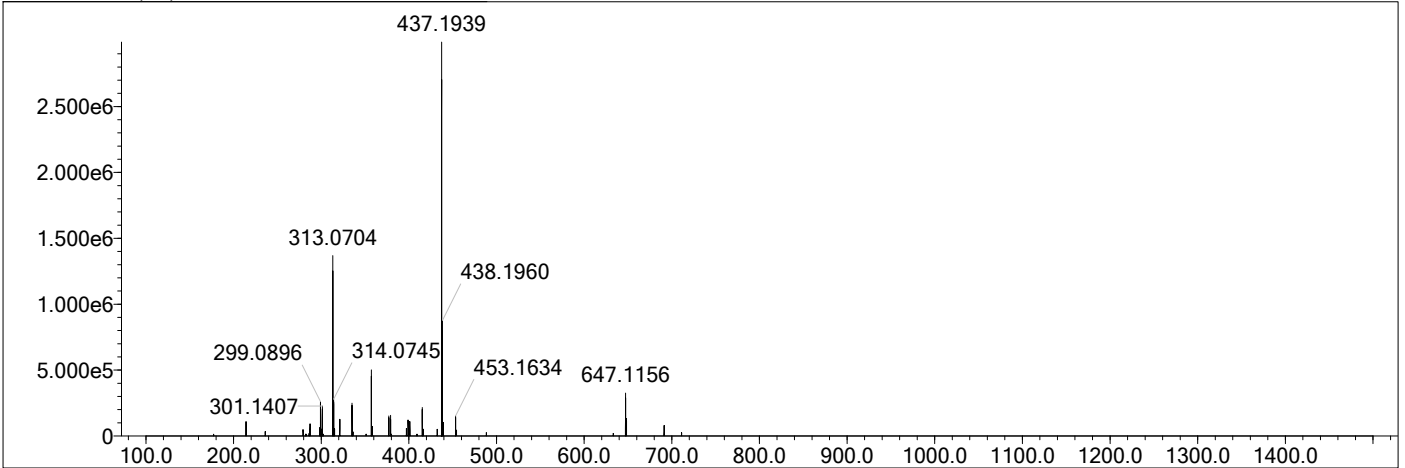
Error Margin (ppm): 100
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

DBE Range: -2.0 - 1000.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

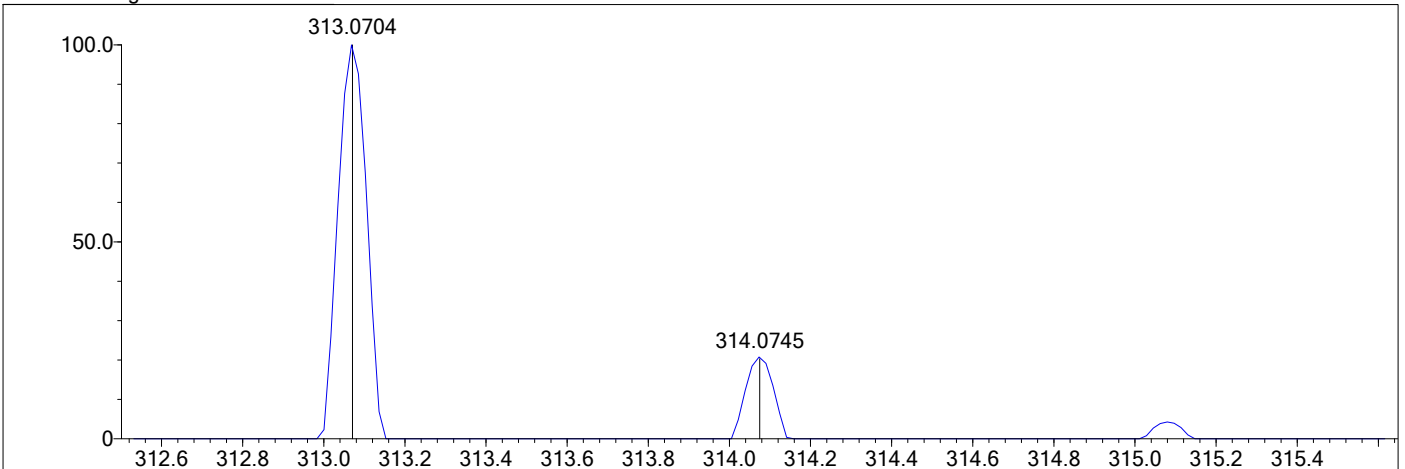
Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

1u

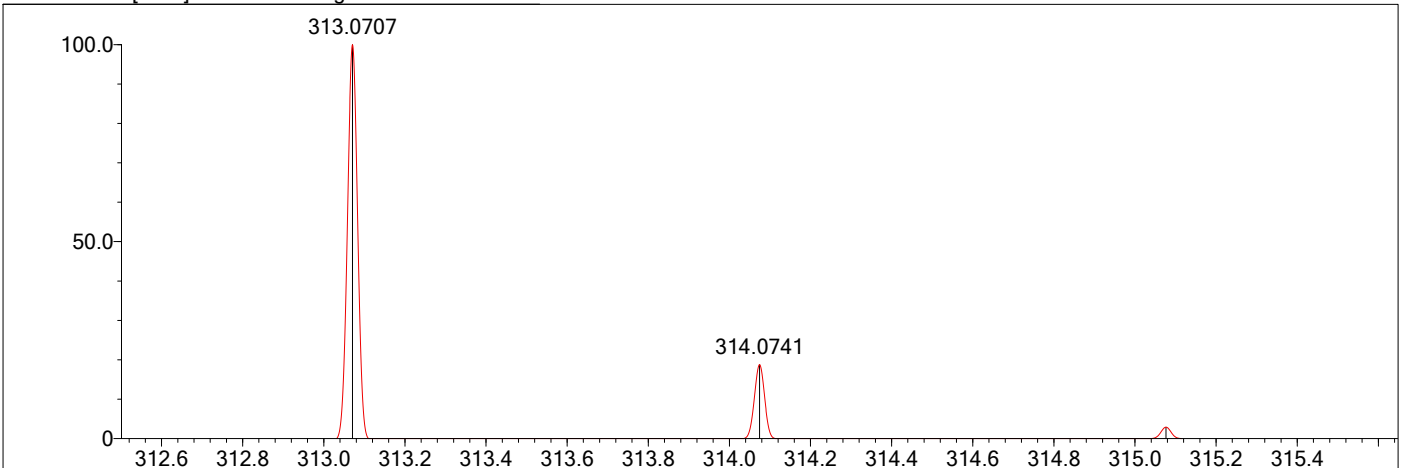
Event#: 1 MS(E+) Ret. Time : 1.240 Scan#: 187



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: F:\高分辨数据\Zouyong\sjf\S18.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					

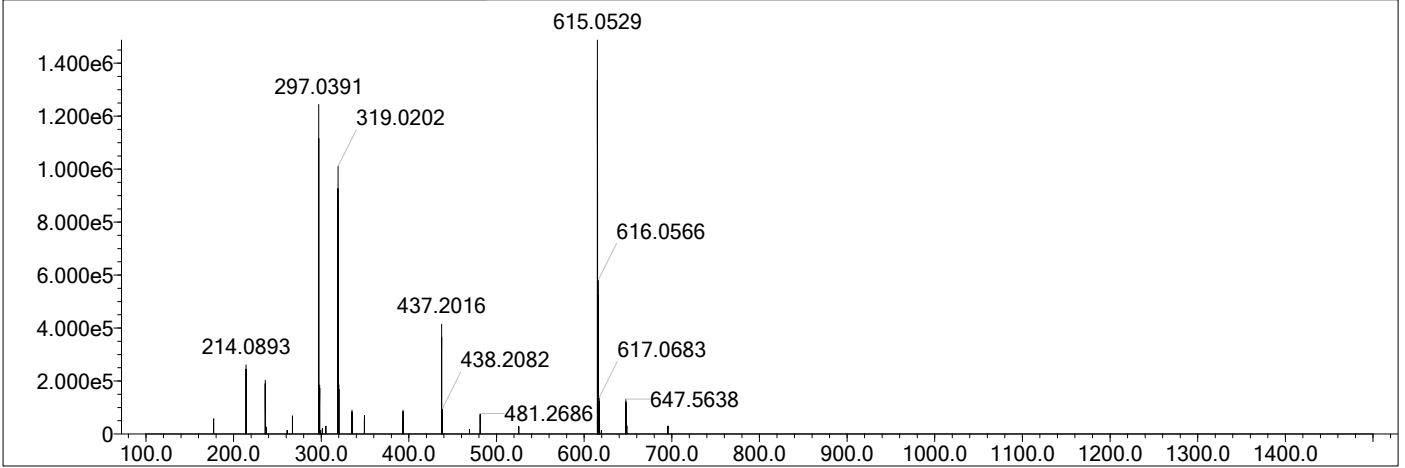
Error Margin (ppm): 100
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

DBE Range: -2.0 - 1000.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

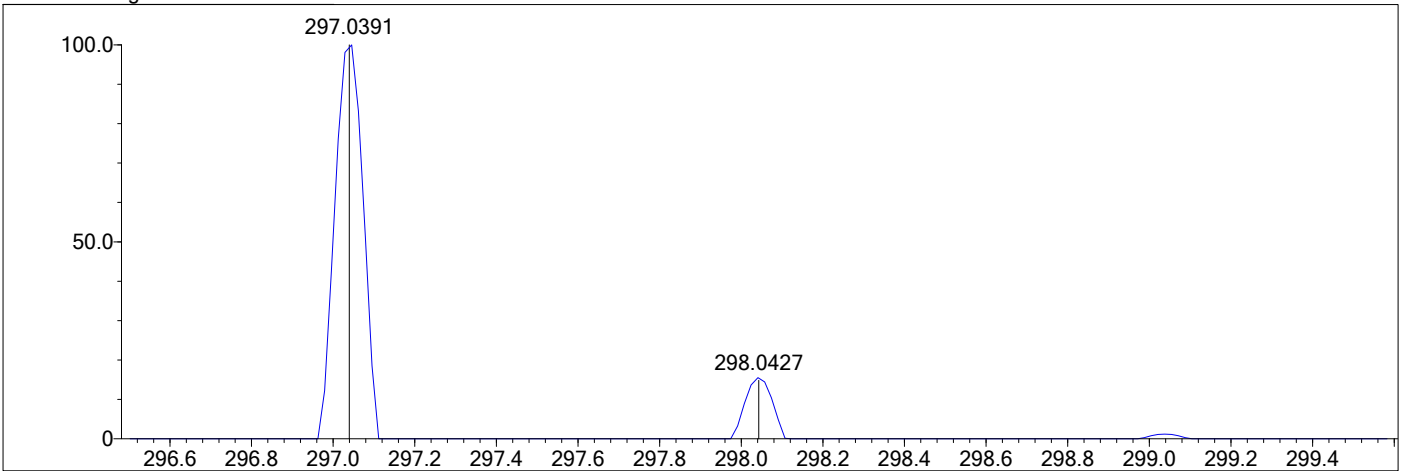
Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

1v

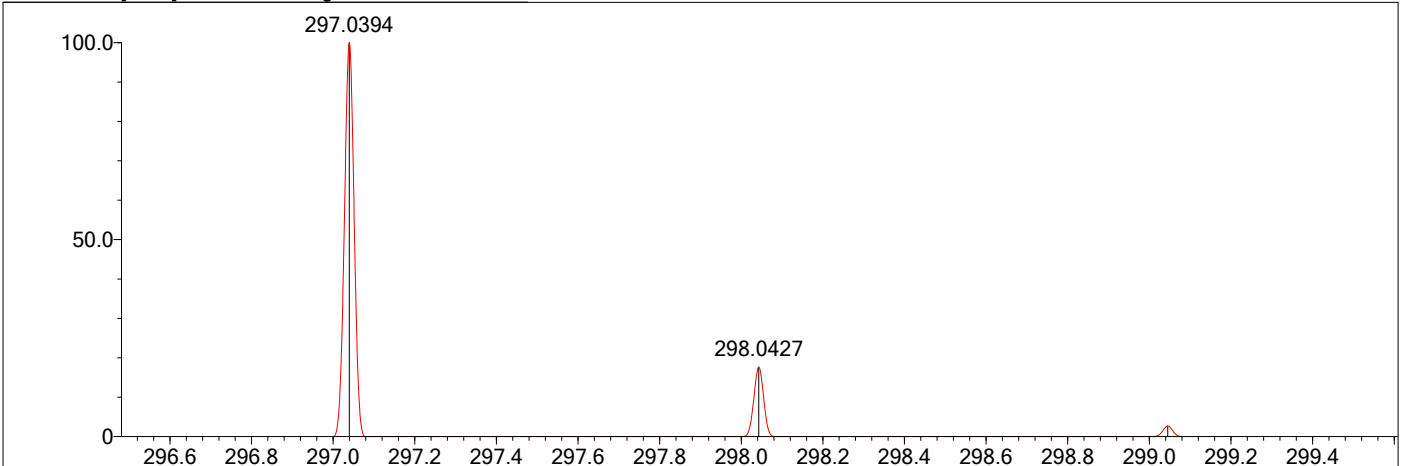
Event#: 1 MS(E+) Ret. Time : 1.200 Scan# : 181



Measured region for 297.0391 m/z



C16 H8 O6 [M+H]⁺ : Predicted region for 297.0394 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	71.95	C16 H8 O6	[M+H] ⁺	297.0391	297.0394	-0.3	-1.01	71.96	13.0

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

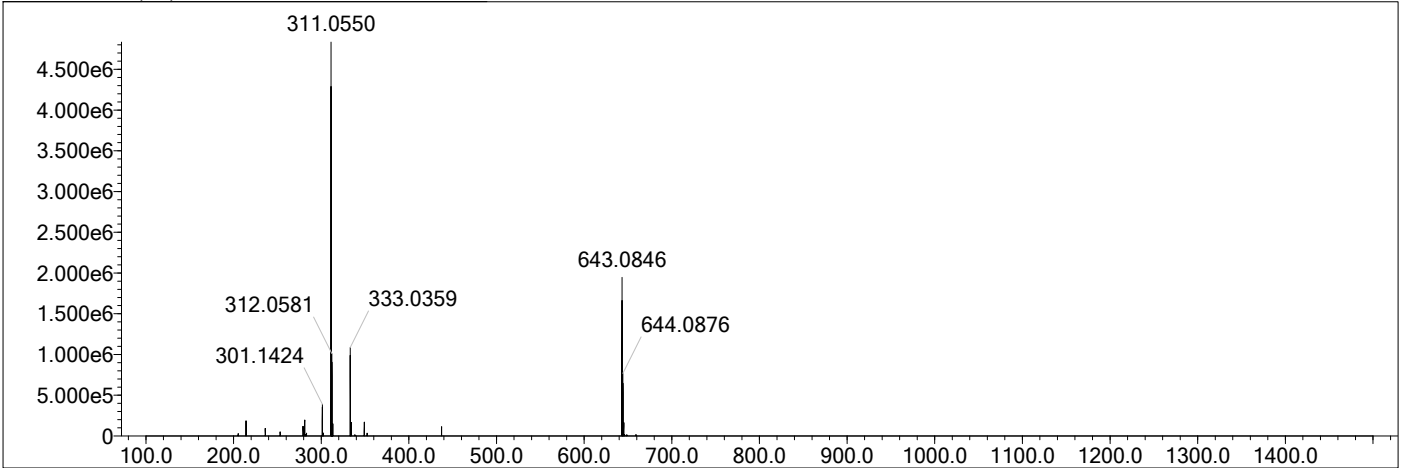
Error Margin (ppm): 100
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

DBE Range: -2.0 - 1000.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

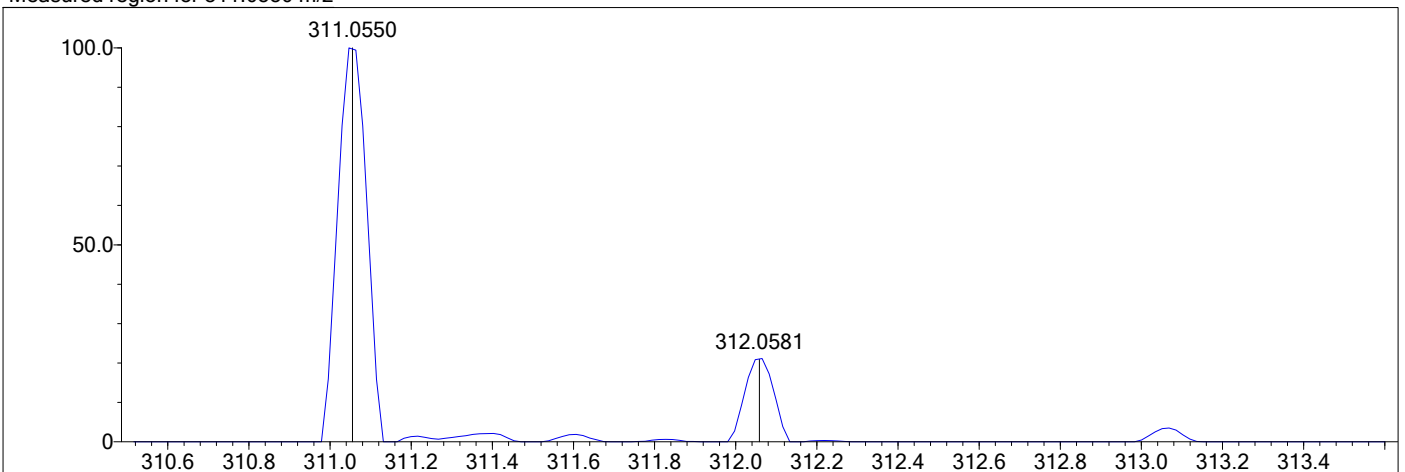
Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

1w

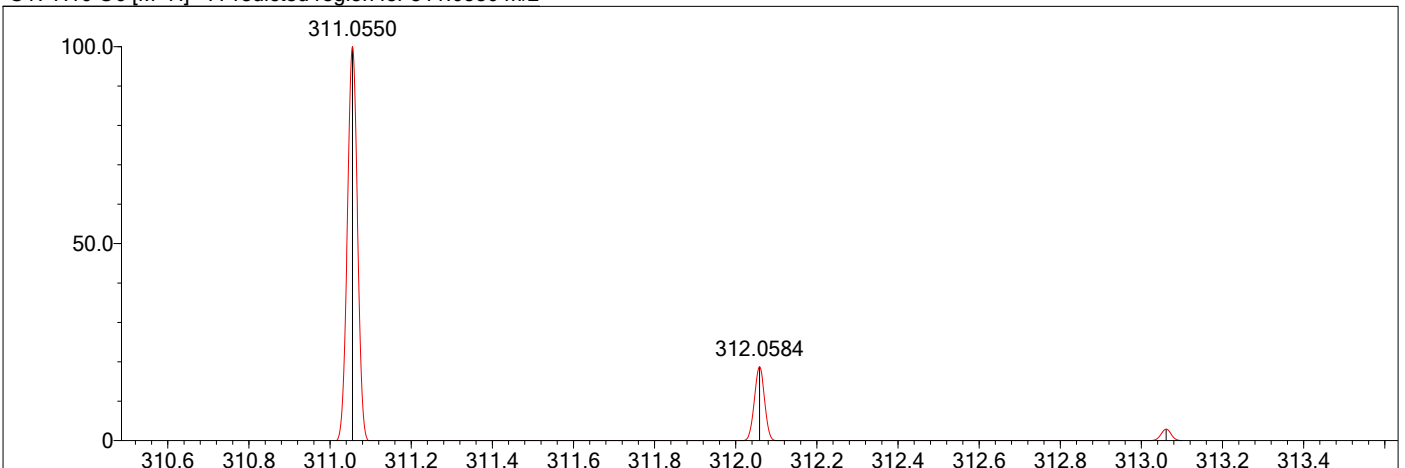
Event#: 1 MS(E+) Ret. Time : 1.413 Scan# : 213



Measured region for 311.0550 m/z



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



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	74.93	C17 H10 O6	[M+H] ⁺	311.0550	311.0550	-0.0	0.00	74.93	13.0

Data File: F:\高分辨数据\Zouyong\sjf\S20.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	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	60	Na	1	0	0	K	1	0	0					
N	3	0	0	Si	4	0	0	Mn	3	0	0					

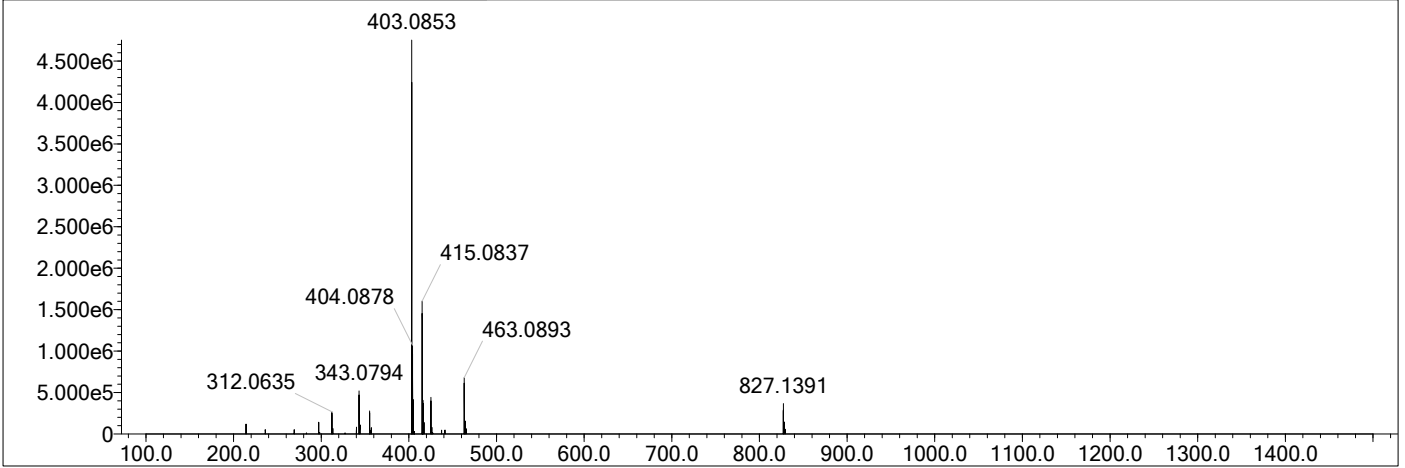
Error Margin (ppm): 100
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

DBE Range: -2.0 - 1000.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

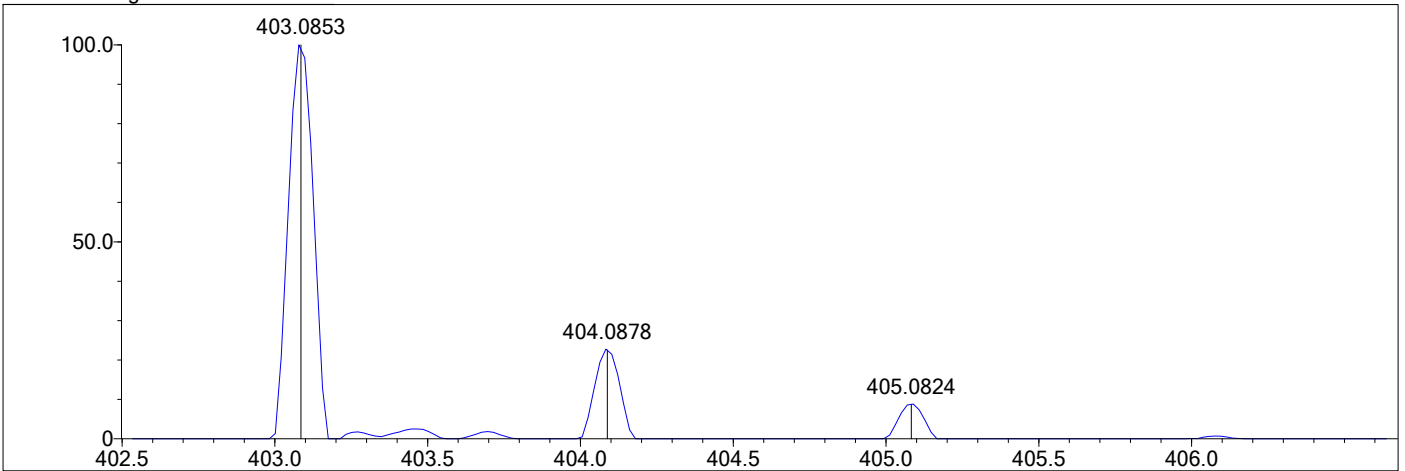
Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

1jj

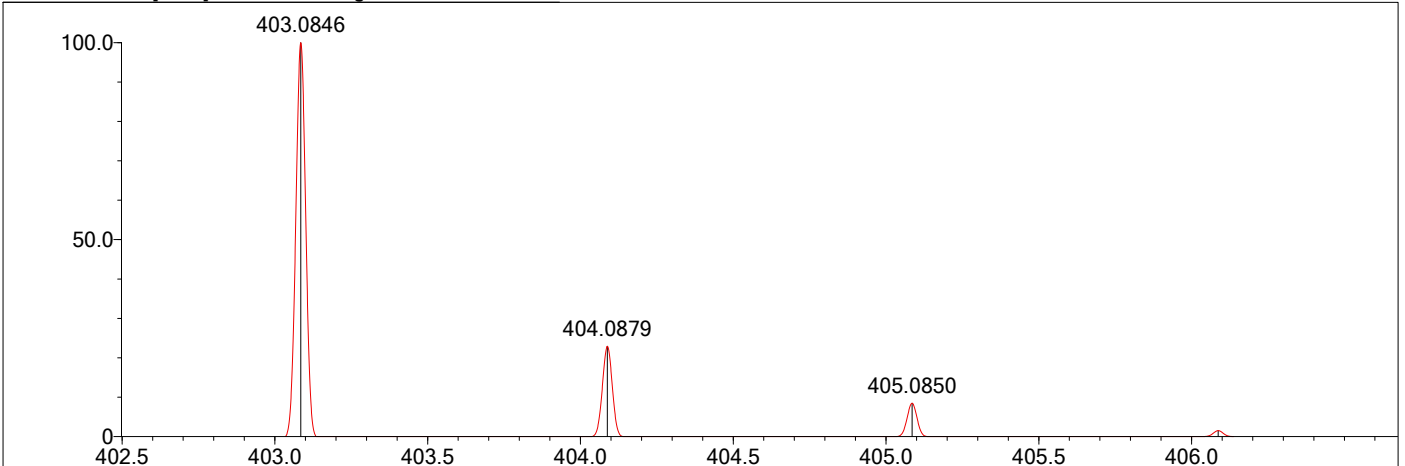
Event#: 1 MS(E+) Ret. Time : 1.240 Scan#: 187



Measured region for 403.0853 m/z



C20 H18 O7 S [M+H]⁺ : Predicted region for 403.0846 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	85.83	C20 H18 O7 S	[M+H] ⁺	403.0853	403.0846	0.7	1.74	87.45	12.0