

Data File: F:\高分辨数据\Zouyong\SXH\SJF-2A.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	10	O	2	0	4	Cl	1	0	0	H
B	3	0	0	F	1	0	0	Br	1	0	0	HCOO
C	4	0	15	P	3	0	0	I	3	0	0	CH3COO
N	3	0	0	S	2	0	0					Cl

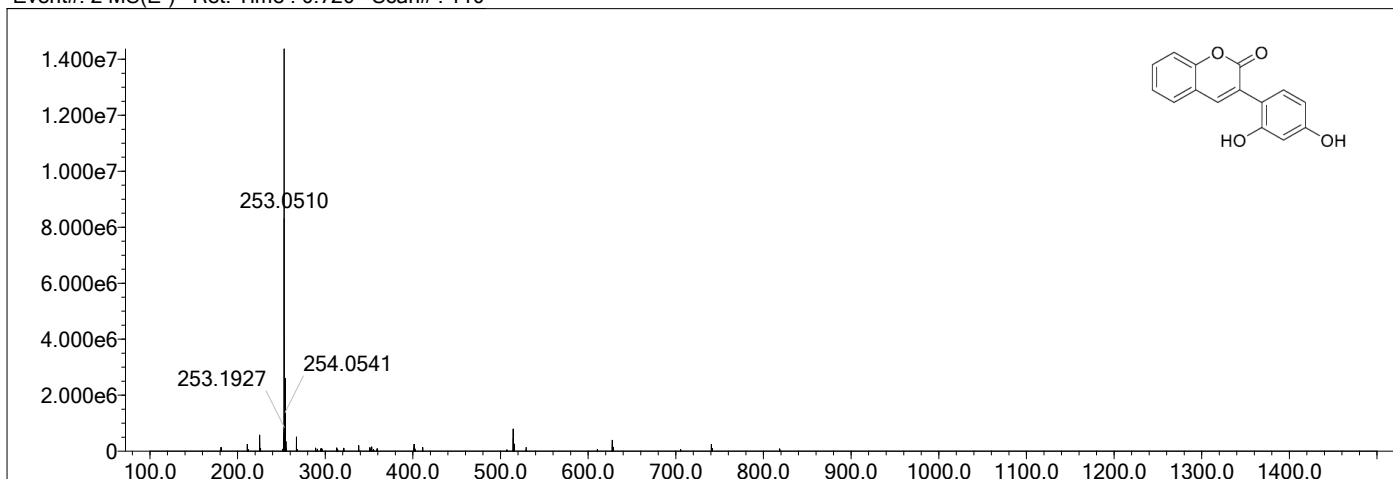
Error Margin (ppm): 5  
 HC Ratio: unlimited  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

DBE Range: -1.0 - 1500.0  
 Apply N Rule: no  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

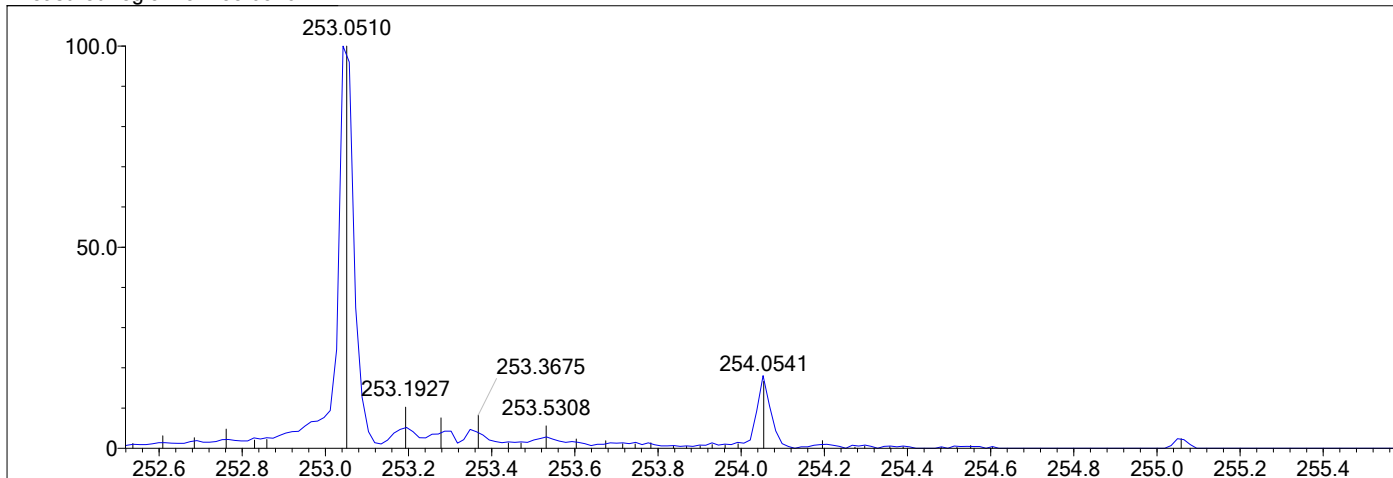
Electron Ions: both  
 Use MSn Info: no  
 Isotope Res: 10000  
 Max Results: 40

2a

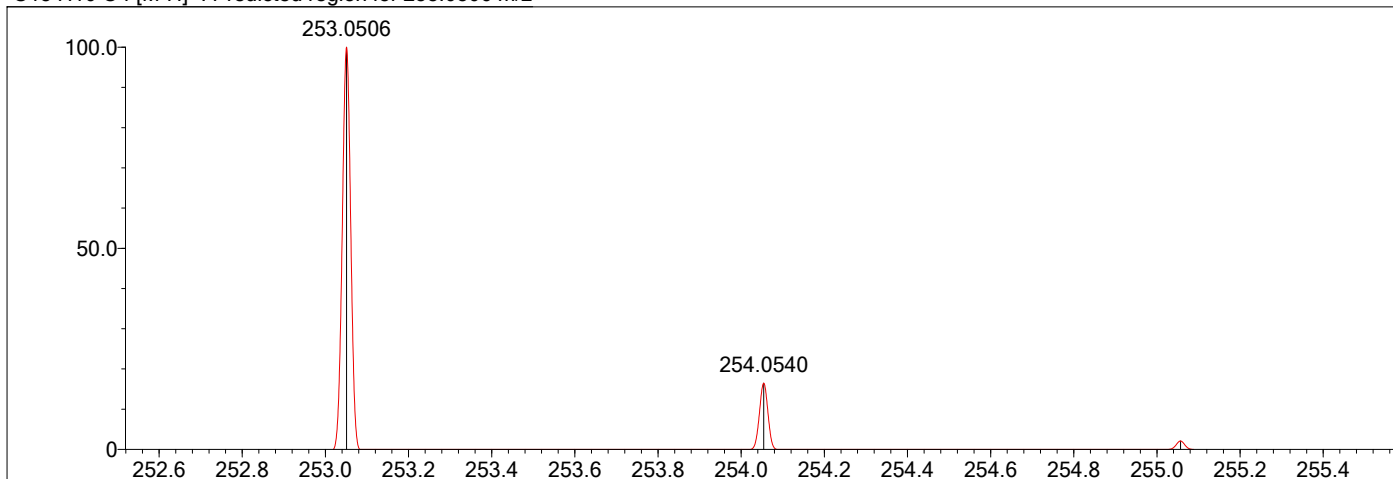
Event#: 2 MS(E-) Ret. Time : 0.720 Scan# : 110



Measured region for 253.0510 m/z



C15 H10 O4 [M-H]- : Predicted region for 253.0506 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	92.22	C15 H10 O4	[M-H]-	253.0510	253.0506	0.4	1.58	93.57	11.0

Data File: F:\高分辨数据\Zouyong\SXH\SJF-2B.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	10	O	2	0	3	Cl	1	0	0	H
B	3	0	0	F	1	0	0	Br	1	0	0	Na
C	4	0	15	P	3	0	0	I	3	0	0	K
N	3	0	0	S	2	0	0					NH4

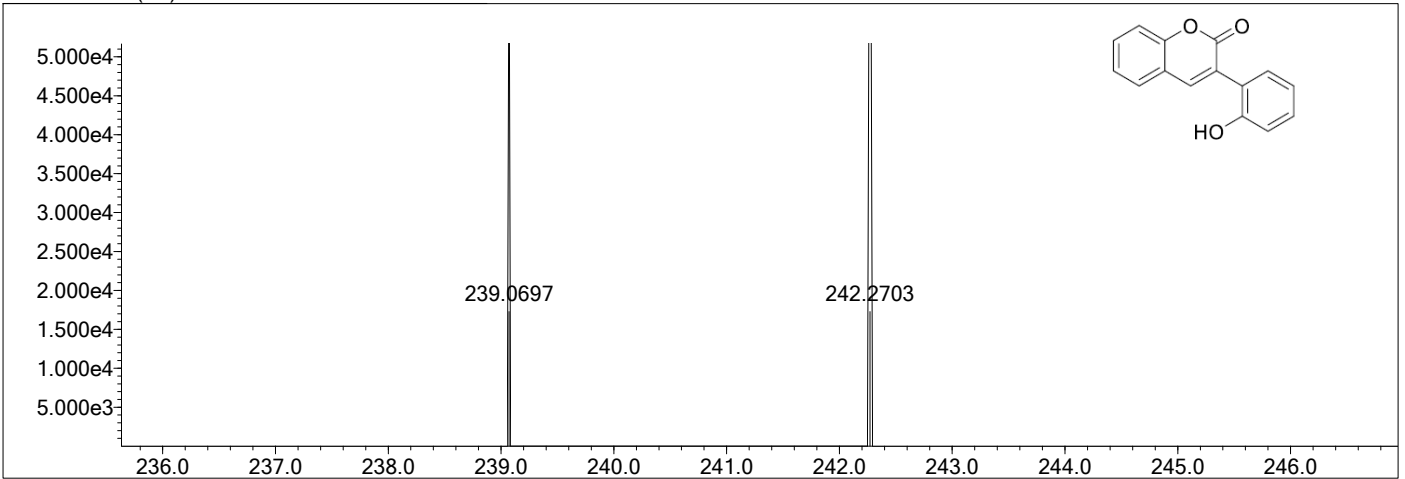
Error Margin (ppm): 5  
 HC Ratio: unlimited  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

DBE Range: -1.0 - 1500.0  
 Apply N Rule: no  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

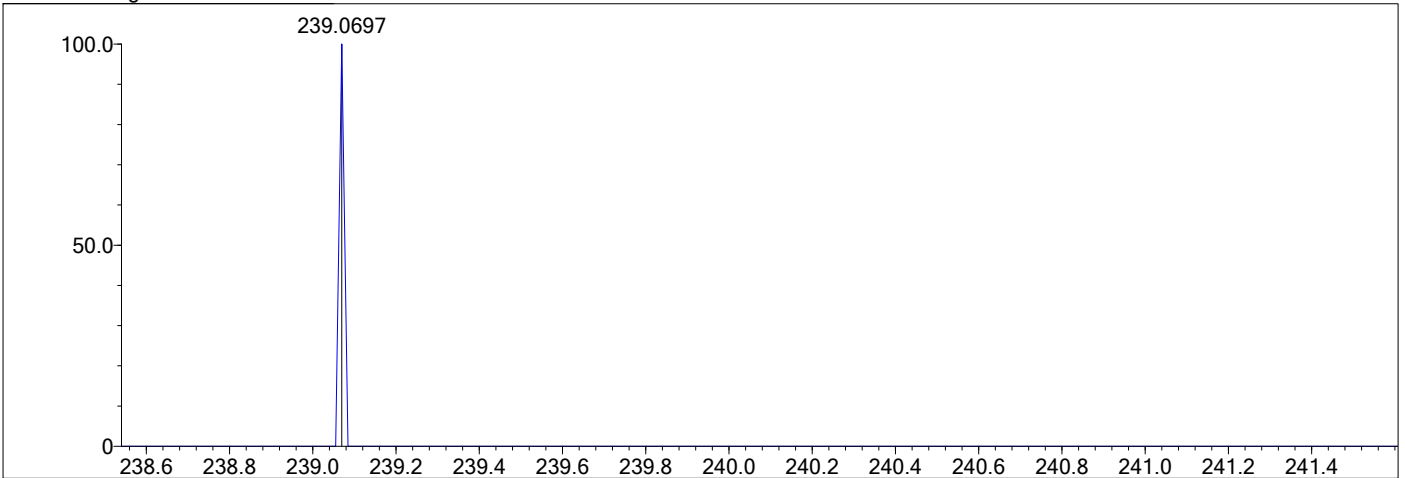
Electron Ions: both  
 Use MSn Info: no  
 Isotope Res: 10000  
 Max Results: 40

Event#: 1 MS(E+) Ret. Time : 0.933 Scan# : 141

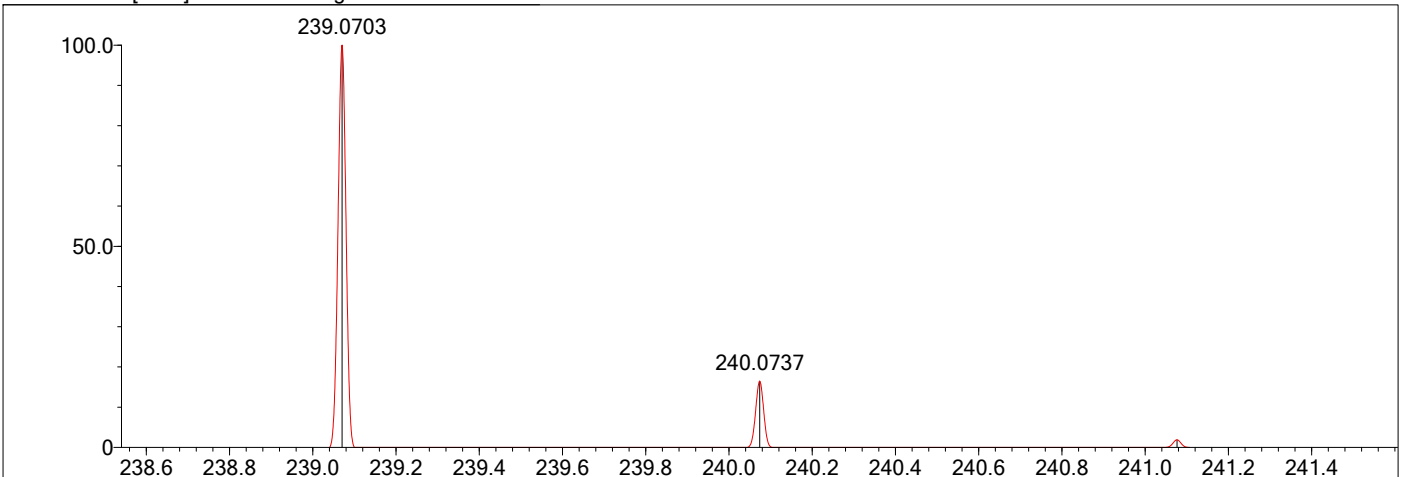
2b



Measured region for 239.0697 m/z



C15 H10 O3 [M+H]+ : Predicted region for 239.0703 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	0.00	C15 H10 O3	[M+H]+	239.0697	239.0703	-0.6	-2.51	0.00	11.0

Data File: \\Deep-20160624\data1\邹永\SXH\SJF-2C.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	7	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	K
B	3	0	0	P	3	0	0	Cu	2	0	0	Au	1	0	0	
C	4	0	30	S	2	0	0	Se	2	0	0					
N	3	0	8	Cl	1	0	0	Br	1	0	0					

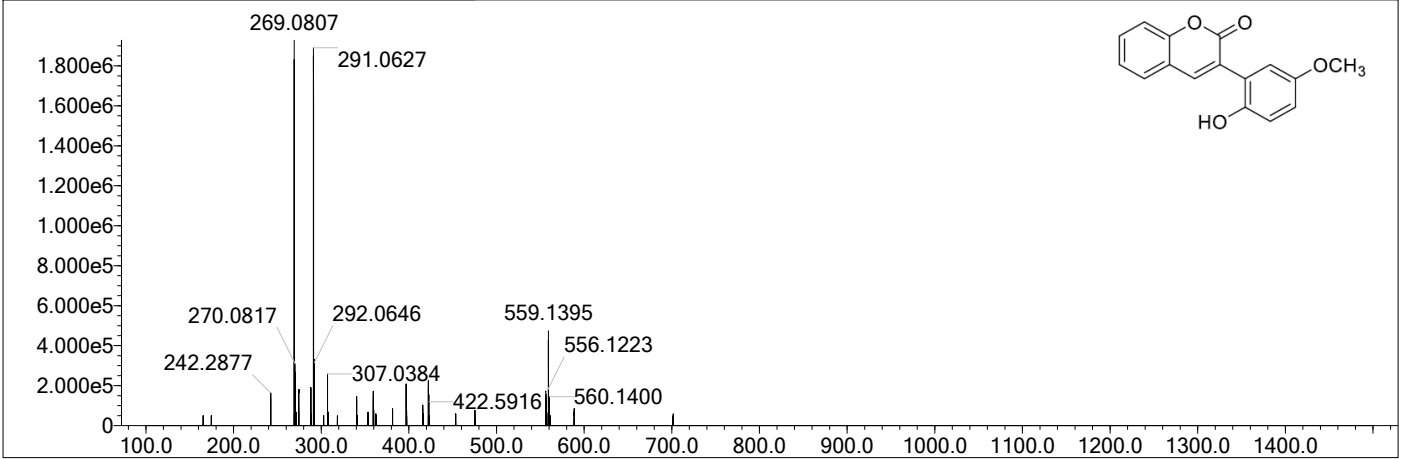
Error Margin (ppm): 50  
 HC Ratio: 0.0 - 20.0  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

DBE Range: -100.0 - 1000.0  
 Apply N Rule: yes  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

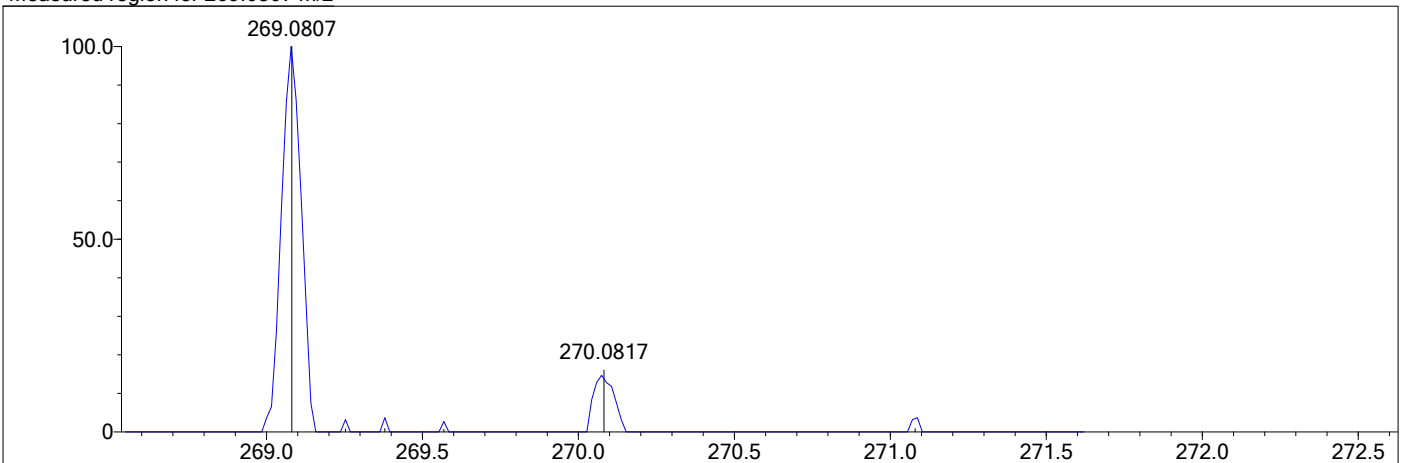
Electron Ions: both  
 Use MSn Info: no  
 Isotope Res: 10000  
 Max Results: 2000

Event#: 1 MS(E+) Ret. Time: 0.160 Scan#: 25

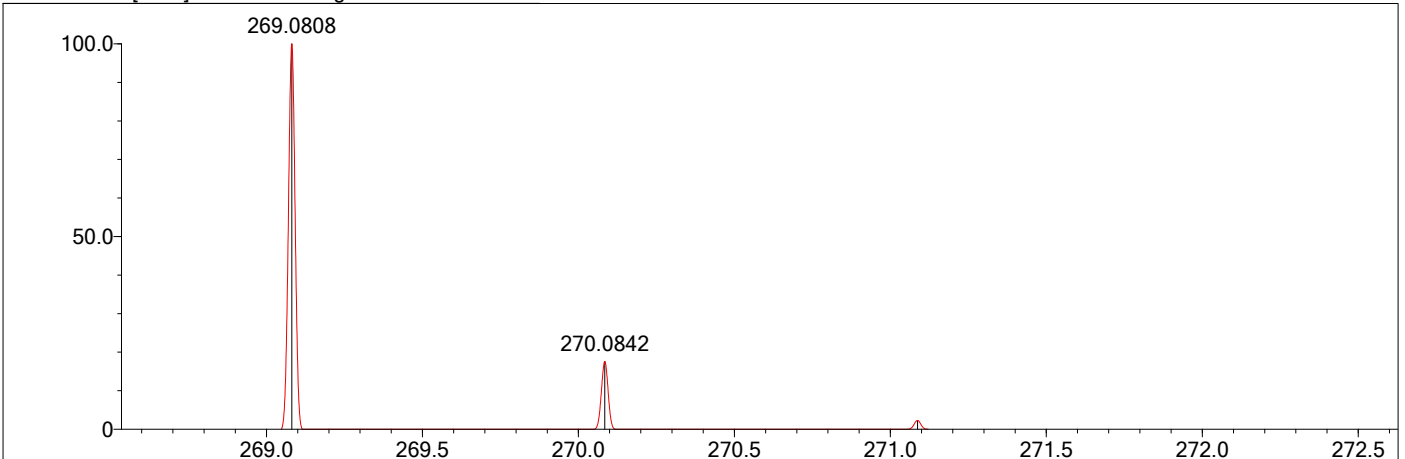
2c



Measured region for 269.0807 m/z



C16 H12 O4 [M+H]<sup>+</sup> : Predicted region for 269.0808 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	64.46	C16 H12 O4	[M+H] <sup>+</sup>	269.0807	269.0808	-0.1	-0.37	64.46	11.0

Data File: \\Deep-20160624\data1\邹永\SXH\SJF-2D.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	7	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	K
B	3	0	0	P	3	0	0	Cu	2	0	0	Au	1	0	0	
C	4	0	30	S	2	0	0	Se	2	0	0					
N	3	0	8	Cl	1	0	0	Br	1	0	0					

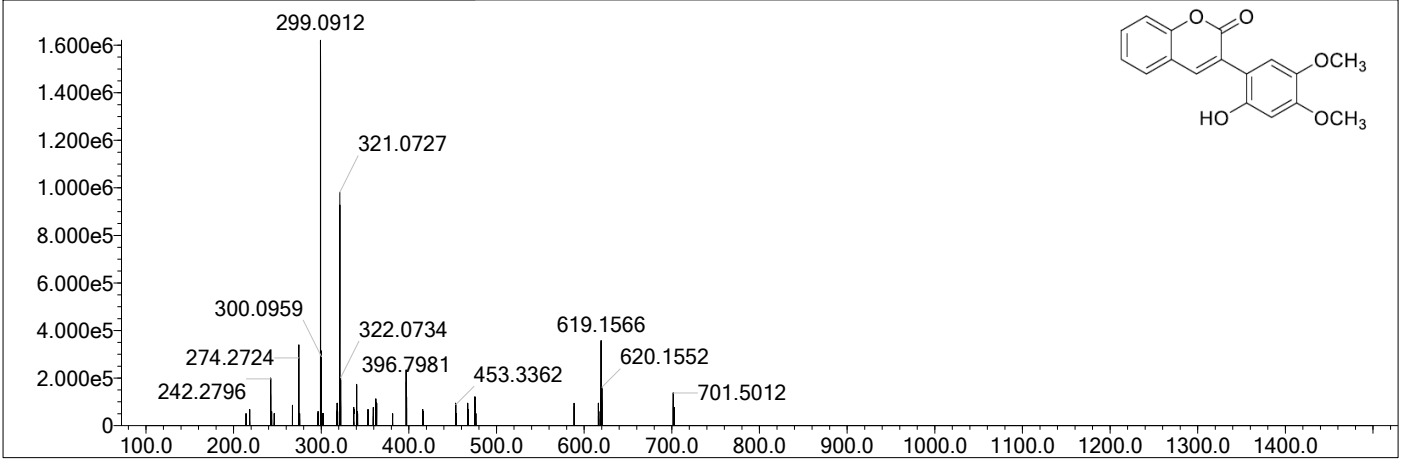
Error Margin (ppm): 50  
 HC Ratio: 0.0 - 20.0  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

DBE Range: -100.0 - 1000.0  
 Apply N Rule: yes  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

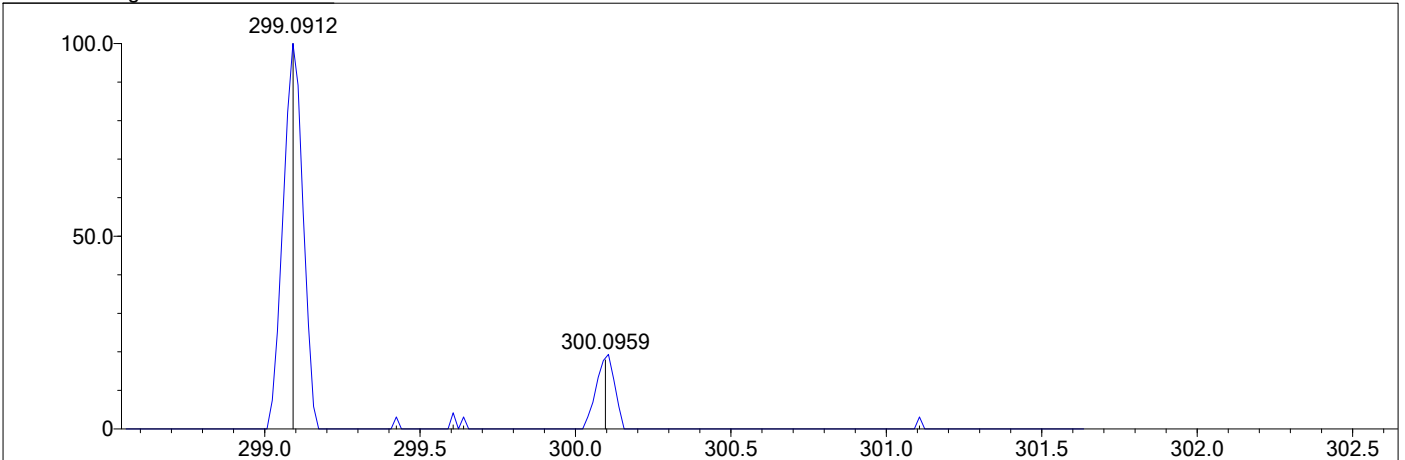
Electron Ions: both  
 Use MSn Info: no  
 Isotope Res: 10000  
 Max Results: 2000

Event#: 1 MS(E+) Ret. Time: 0.147 Scan#: 23

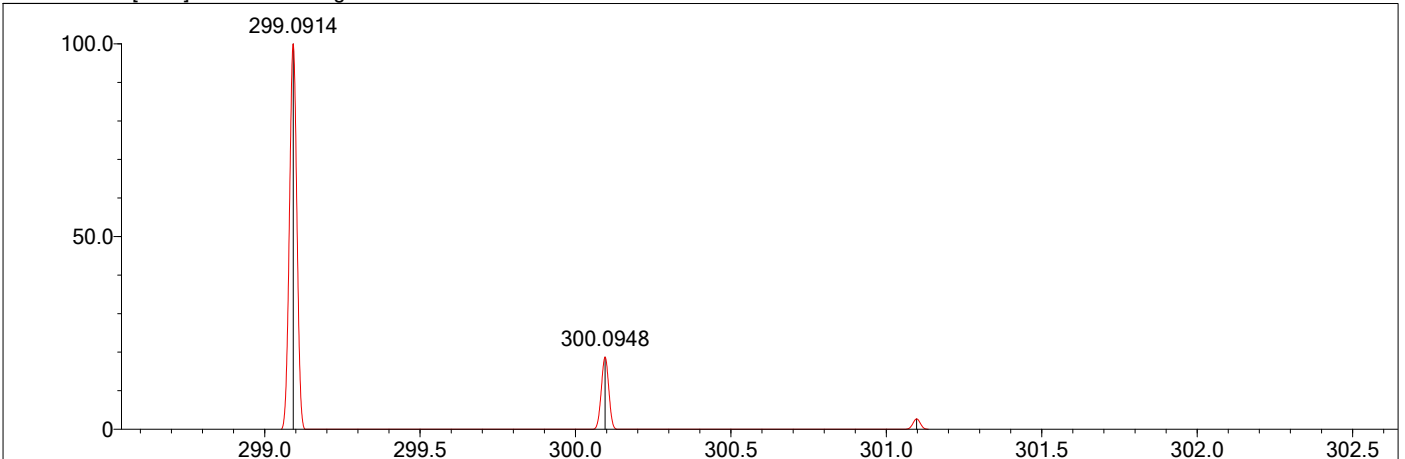
2d



Measured region for 299.0912 m/z



C17 H14 O5 [M+H]+ : Predicted region for 299.0914 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	69.34	C17 H14 O5	[M+H]+	299.0912	299.0914	-0.2	-0.67	69.34	11.0

Data File: \\Deep-20160624\data1\邹永\SXH\SJF-2E.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	7	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	K
B	3	0	0	P	3	0	0	Cu	2	0	0	Au	1	0	0	
C	4	0	30	S	2	0	0	Se	2	0	0					
N	3	0	8	Cl	1	0	0	Br	1	0	0					

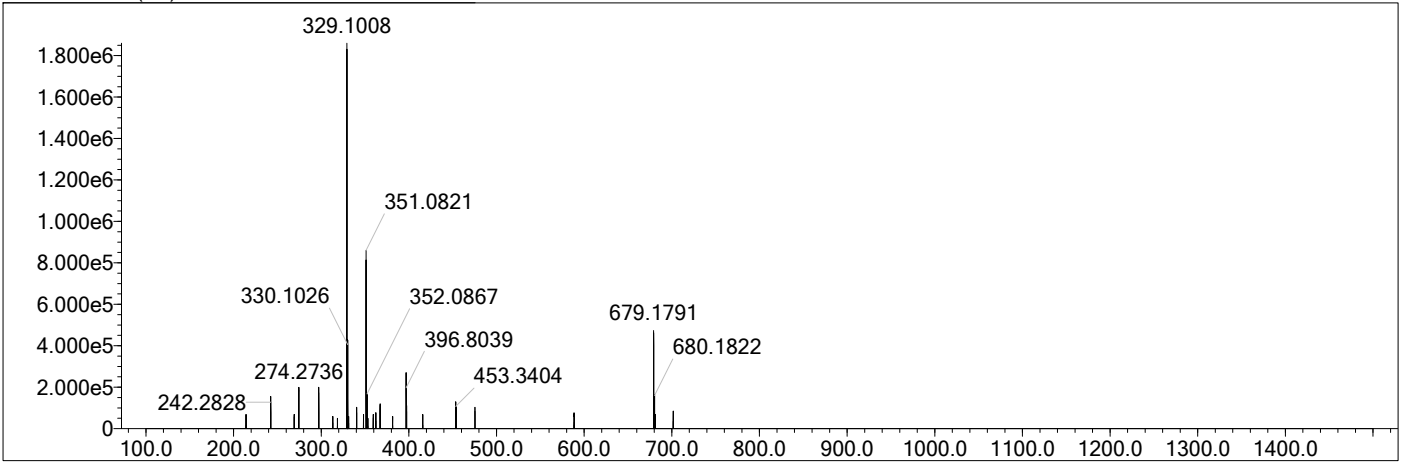
Error Margin (ppm): 50  
 HC Ratio: 0.0 - 20.0  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

DBE Range: -100.0 - 1000.0  
 Apply N Rule: yes  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

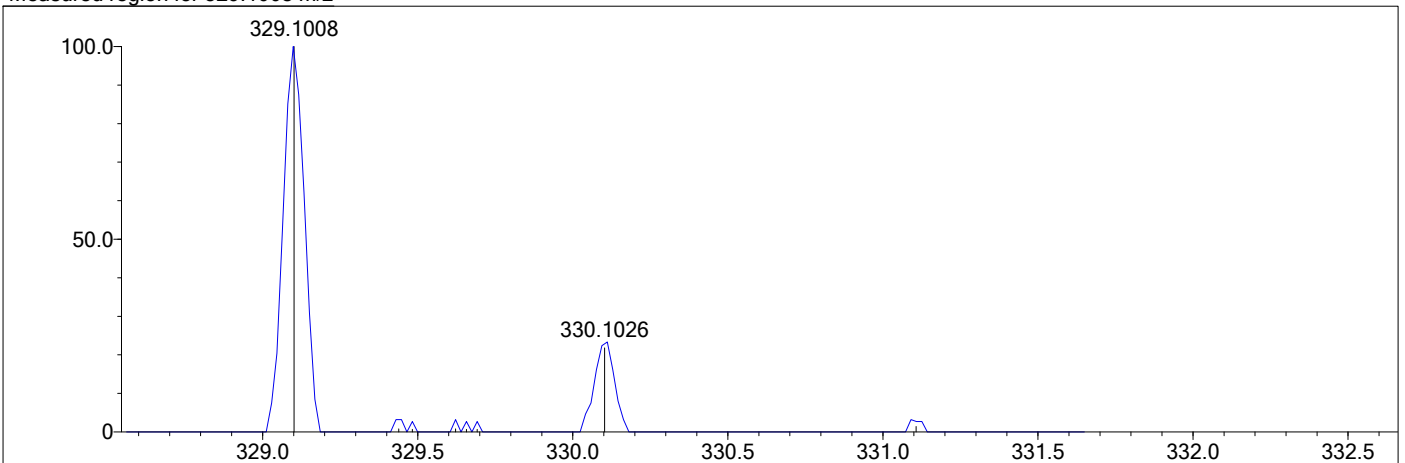
Electron Ions: both  
 Use MSn Info: no  
 Isotope Res: 10000  
 Max Results: 2000

Event#: 1 MS(E+) Ret. Time : 0.173 Scan#: 27

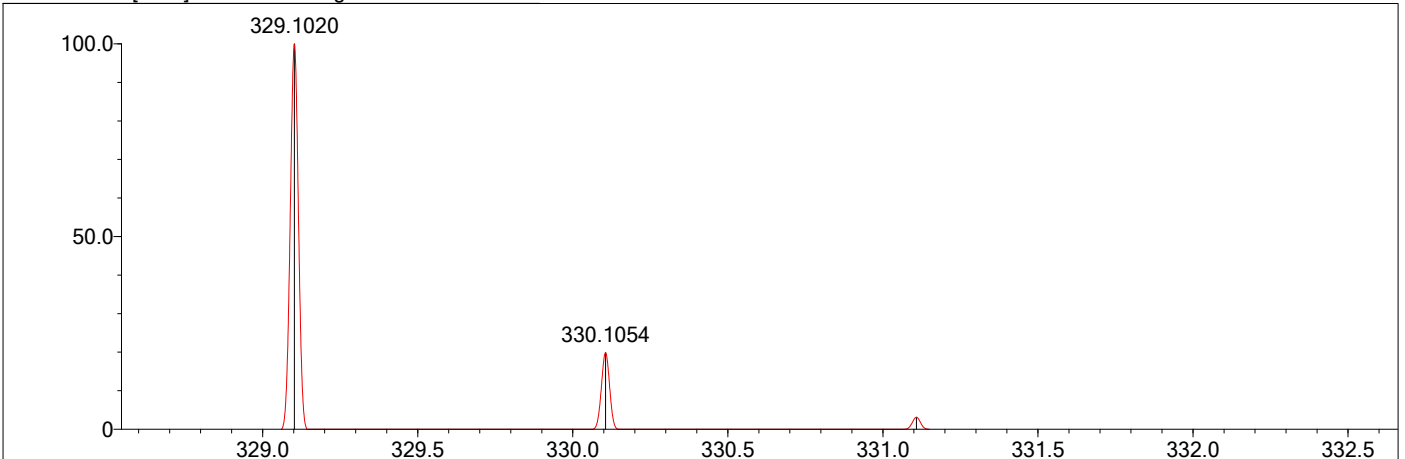
2e



Measured region for 329.1008 m/z



C18 H16 O6 [M+H]+ : Predicted region for 329.1020 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	71.16	C18 H16 O6	[M+H]+	329.1008	329.1020	-1.2	-3.65	76.21	11.0

Data File: \\Deep-20160624\id\data1\邹永\SXH\SJF-2F.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	7	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	K
B	3	0	0	P	3	0	0	Cu	2	0	0	Au	1	0	0	
C	4	0	30	S	2	0	0	Se	2	0	0					
N	3	0	8	Cl	1	0	0	Br	1	0	0					

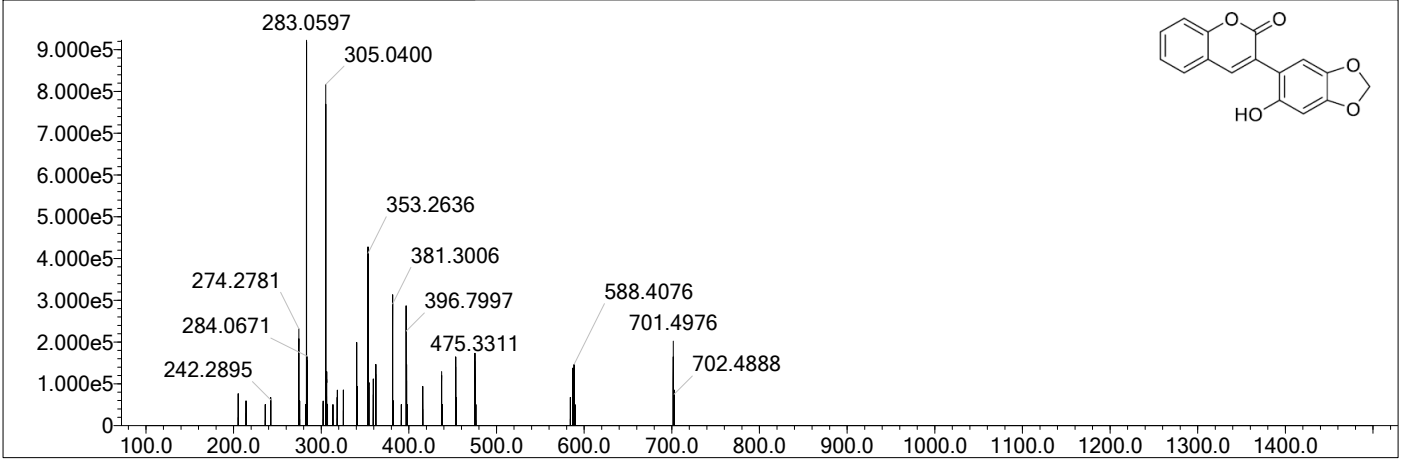
Error Margin (ppm): 50  
 HC Ratio: 0.0 - 20.0  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

DBE Range: -100.0 - 1000.0  
 Apply N Rule: yes  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

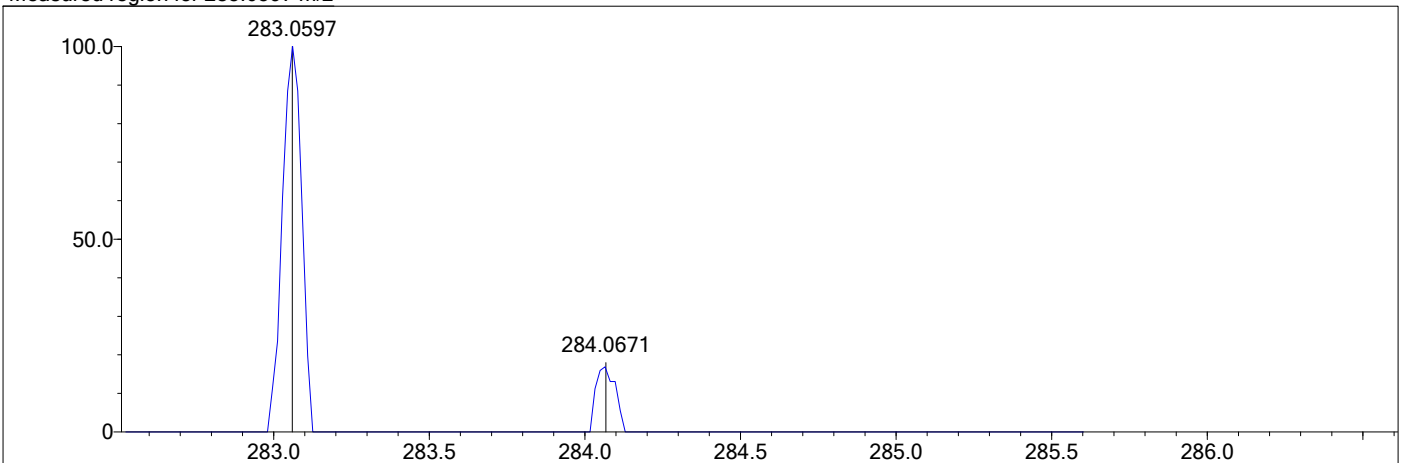
Electron Ions: both  
 Use MSn Info: no  
 Isotope Res: 10000  
 Max Results: 2000

Event#: 1 MS(E+) Ret. Time: 0.200 Scan#: 31

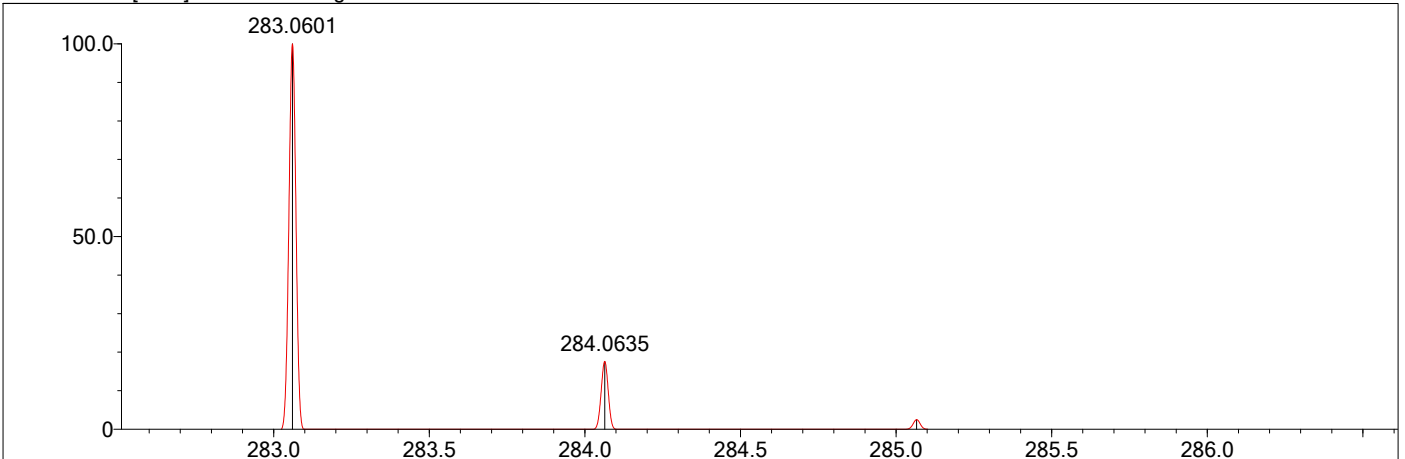
2f



Measured region for 283.0597 m/z



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



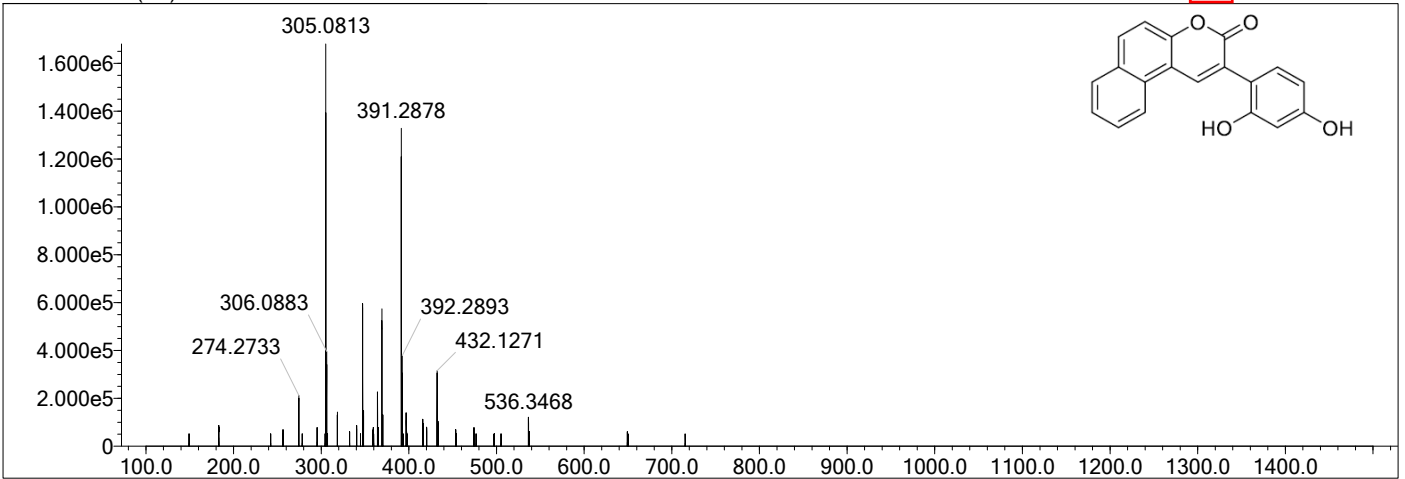
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	81.11	C16 H10 O5	[M+H]+	283.0597	283.0601	-0.4	-1.41	81.95	12.0

Data File: F:\高分辨数据\Zouyong\SXH\SJF-2G.lcd

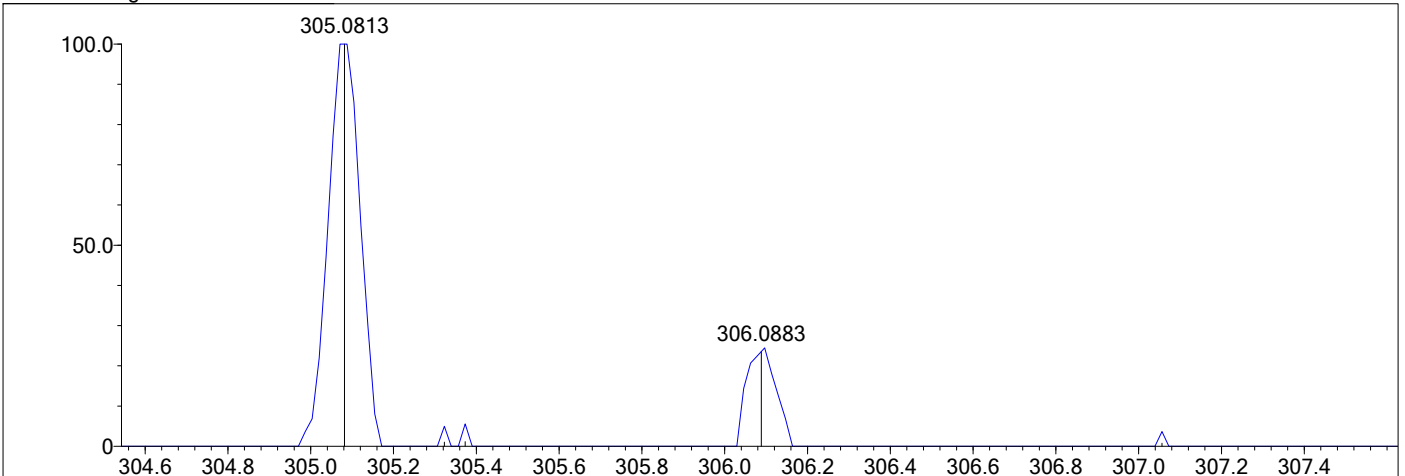
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	12	O	2	0	4	Cl	1	0	0	H
B	3	0	0	F	1	0	0	Br	1	0	0	Na
C	4	0	19	P	3	0	0	I	3	0	0	K
N	3	0	0	S	2	0	0					NH4

Error Margin (ppm): 5  
 DBE Range: -1.0 - 1500.0  
 Electron Ions: both  
 HC Ratio: unlimited  
 Apply N Rule: no  
 Use MSn Info: no  
 Max Isotopes: all  
 Isotope RI (%): 1.00  
 Isotope Res: 10000  
 MSn Iso RI (%): 75.00  
 MSn Logic Mode: AND  
 Max Results: 40

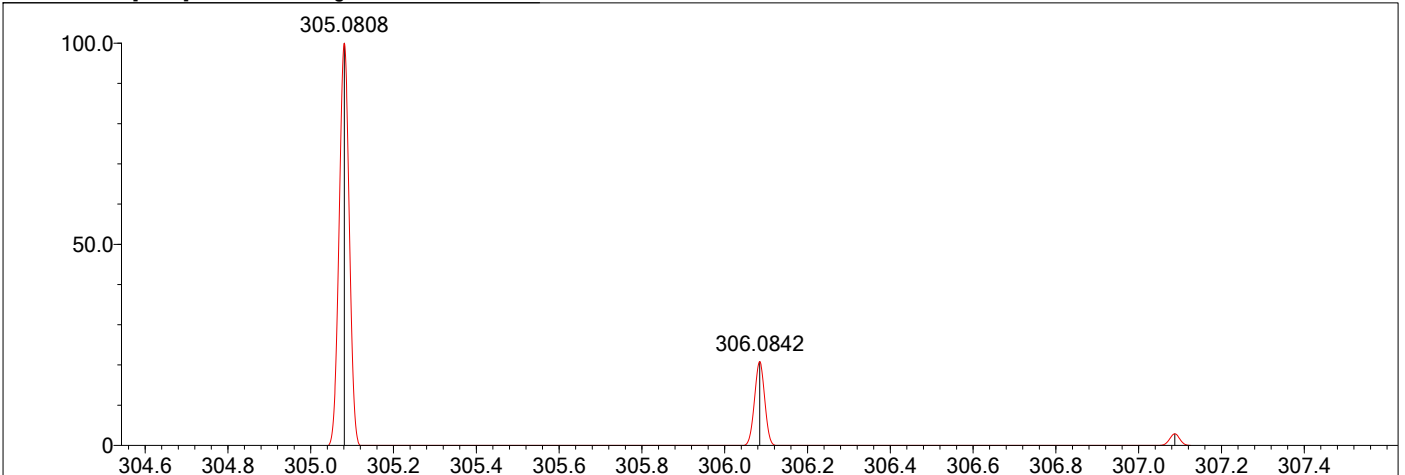
Event#: 1 MS(E+) Ret. Time: 0.773 Scan#: 117



Measured region for 305.0813 m/z



C19 H12 O4 [M+H]<sup>+</sup> : Predicted region for 305.0808 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	77.68	C19 H12 O4	[M+H] <sup>+</sup>	305.0813	305.0808	0.5	1.64	78.95	14.0

Data File: F:\高分辨数据\Zouyong\SXH\SJF-2H.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	10	O	2	0	4	Cl	1	0	0	H
B	3	0	0	F	1	0	0	Br	1	0	0	Na
C	4	0	15	P	3	0	0	I	3	0	0	K
N	3	0	0	S	2	0	0					NH4

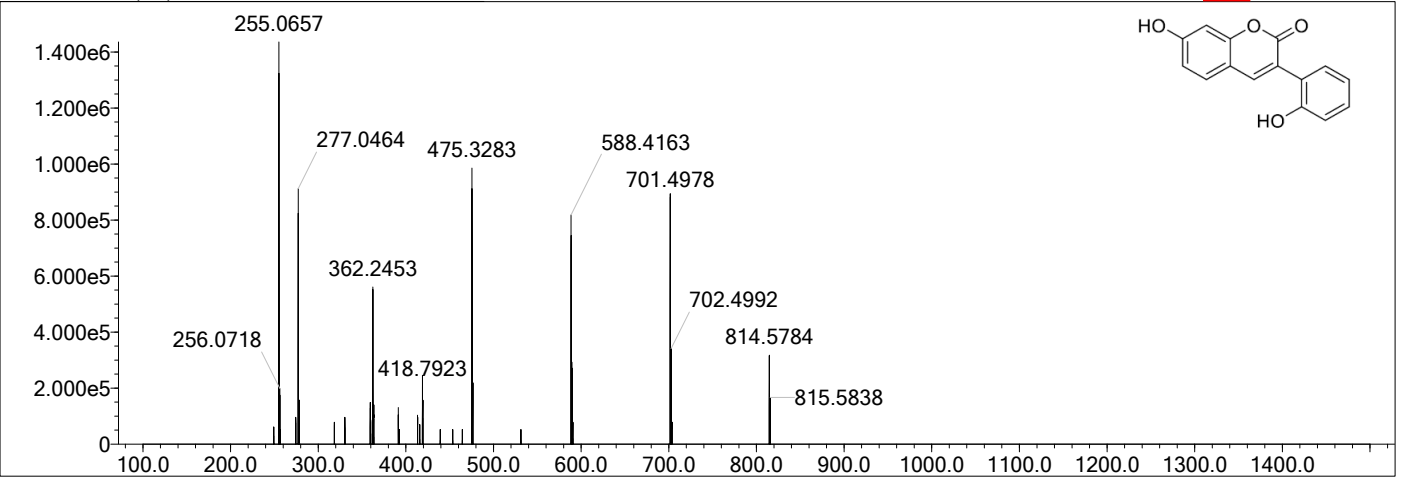
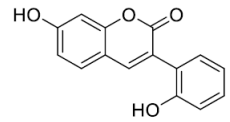
Error Margin (ppm): 5  
 HC Ratio: unlimited  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

DBE Range: -1.0 - 1500.0  
 Apply N Rule: no  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

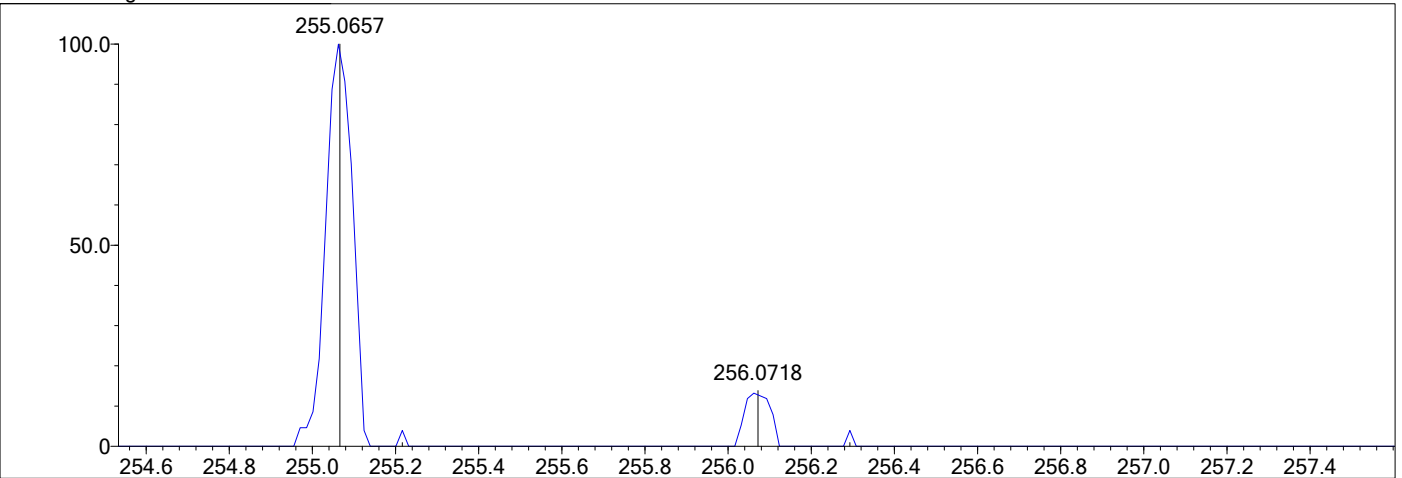
Electron Ions: both  
 Use MSn Info: no  
 Isotope Res: 10000  
 Max Results: 40

Event#: 1 MS(E+) Ret. Time : 0.747 Scan# : 113

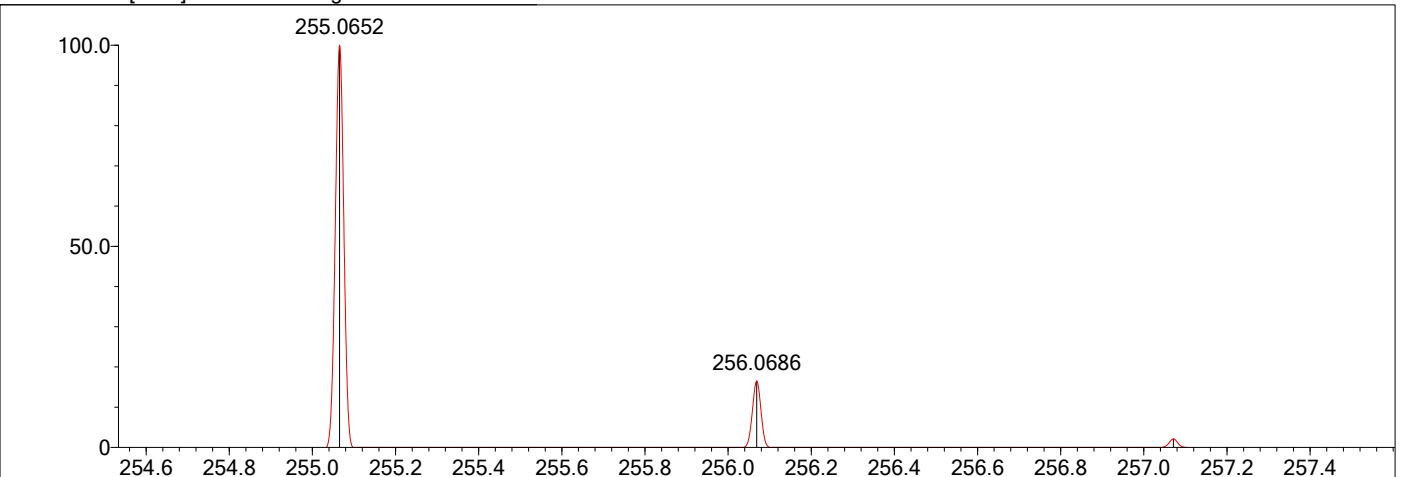
2h



Measured region for 255.0657 m/z



C15 H10 O4 [M+H]<sup>+</sup> : Predicted region for 255.0652 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	67.70	C15 H10 O4	[M+H] <sup>+</sup>	255.0657	255.0652	0.5	1.96	69.36	11.0



Data File: F:\高分辨数据\Zouyong\SXH\SJF-2I.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	12	O	2	0	5	Cl	1	0	0	H
B	3	0	0	F	1	0	0	Br	1	0	0	Na
C	4	0	16	P	3	0	0	I	3	0	0	K
N	3	0	0	S	2	0	0					NH4

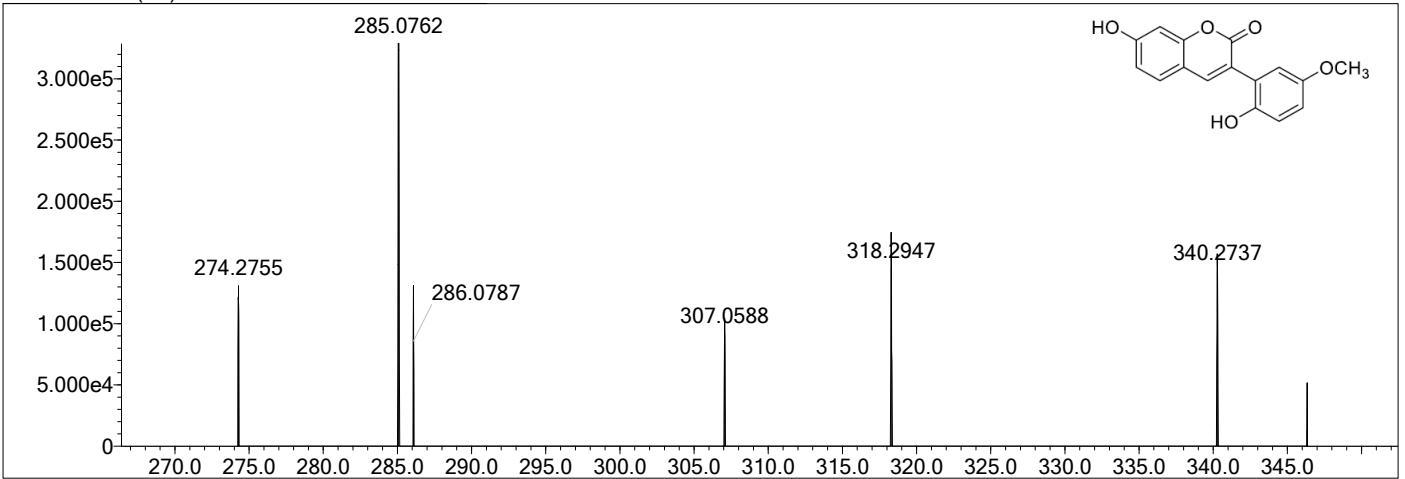
Error Margin (ppm): 5  
 HC Ratio: unlimited  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

DBE Range: -1.0 - 1500.0  
 Apply N Rule: no  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

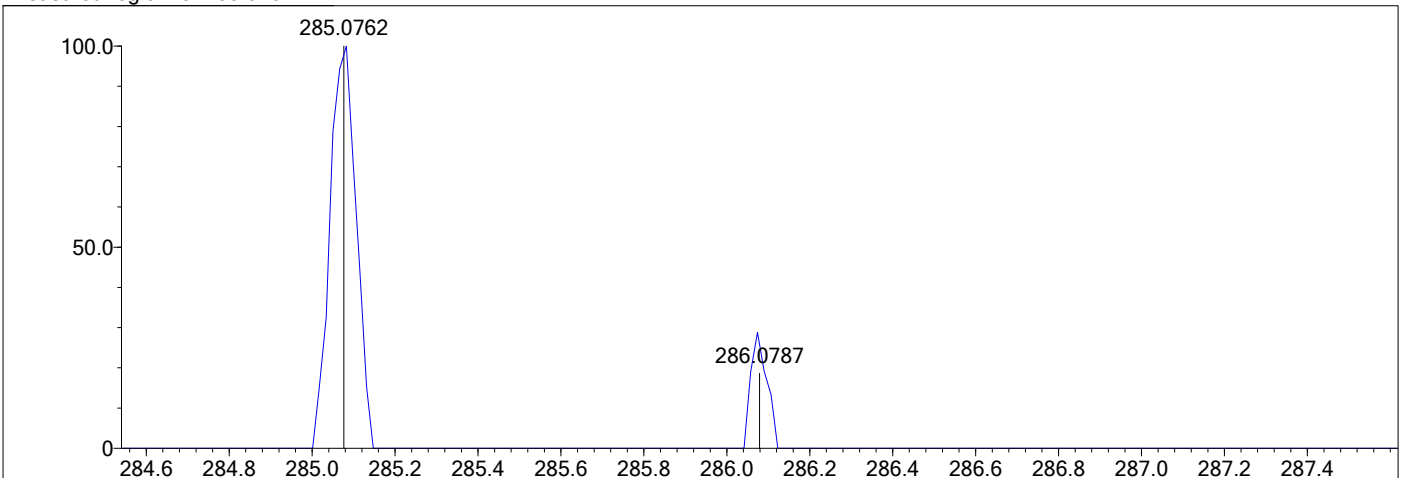
Electron Ions: both  
 Use MSn Info: no  
 Isotope Res: 10000  
 Max Results: 40

Event#: 1 MS(E+) Ret. Time : 0.707 Scan# : 107

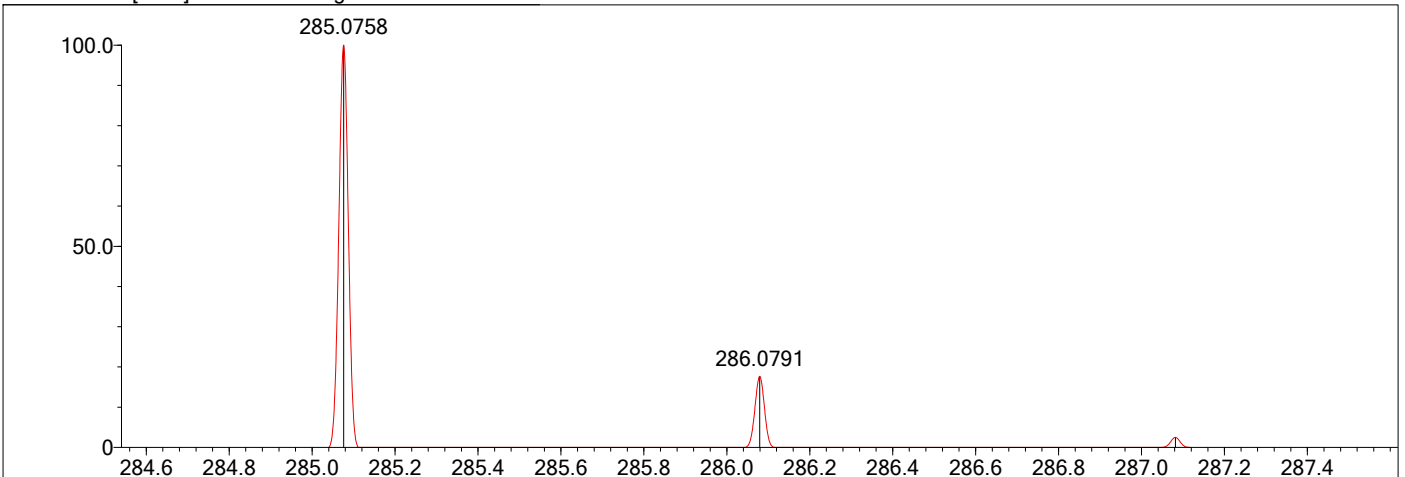
2i



Measured region for 285.0762 m/z



C16 H12 O5 [M+H]<sup>+</sup> : Predicted region for 285.0758 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	53.16	C16 H12 O5	[M+H] <sup>+</sup>	285.0762	285.0758	0.4	1.40	53.70	11.0

Data File: \\Deep-20160624\data1\邹永\SXH\SJF-2J.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	7	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	K
B	3	0	0	P	3	0	0	Cu	2	0	0	Au	1	0	0	
C	4	0	30	S	2	0	0	Se	2	0	0					
N	3	0	8	Cl	1	0	0	Br	1	0	0					

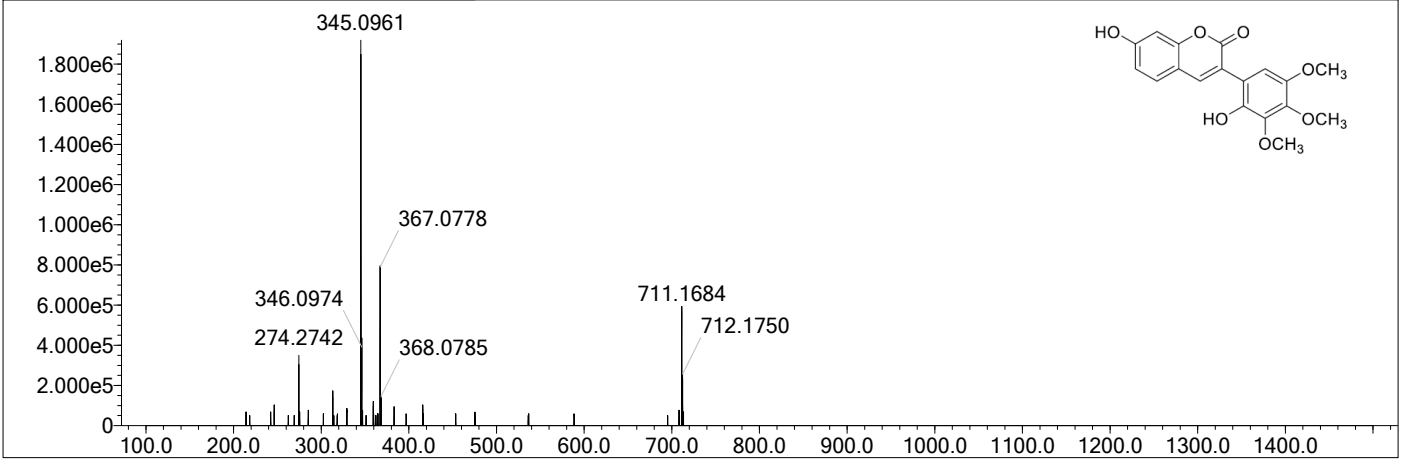
Error Margin (ppm): 50  
 HC Ratio: 0.0 - 20.0  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

DBE Range: -100.0 - 1000.0  
 Apply N Rule: yes  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

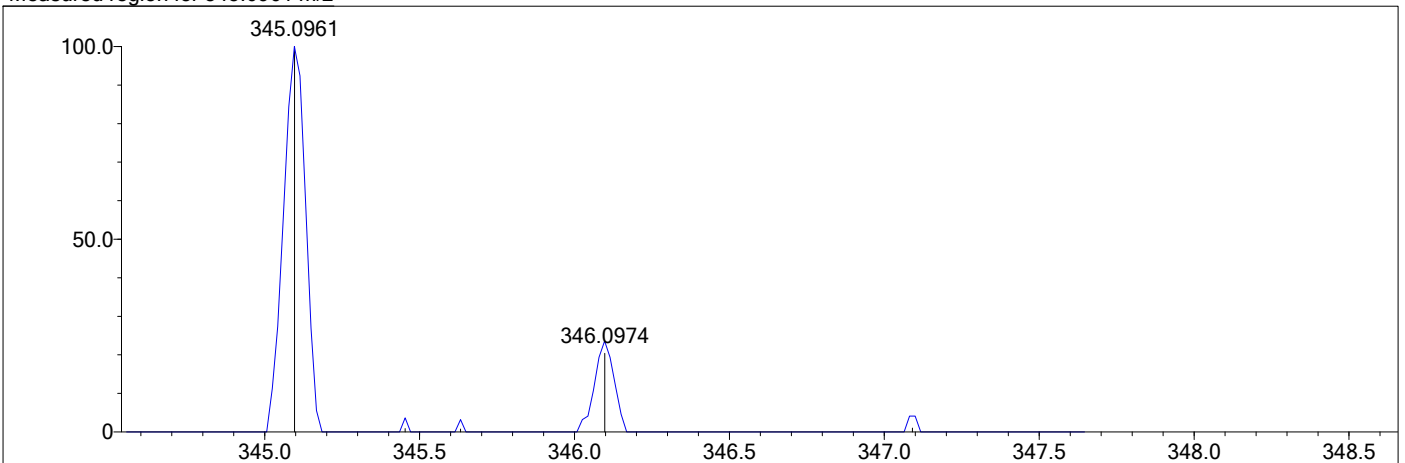
Electron Ions: both  
 Use MSn Info: no  
 Isotope Res: 10000  
 Max Results: 2000

Event#: 1 MS(E+) Ret. Time : 0.120 Scan# : 19

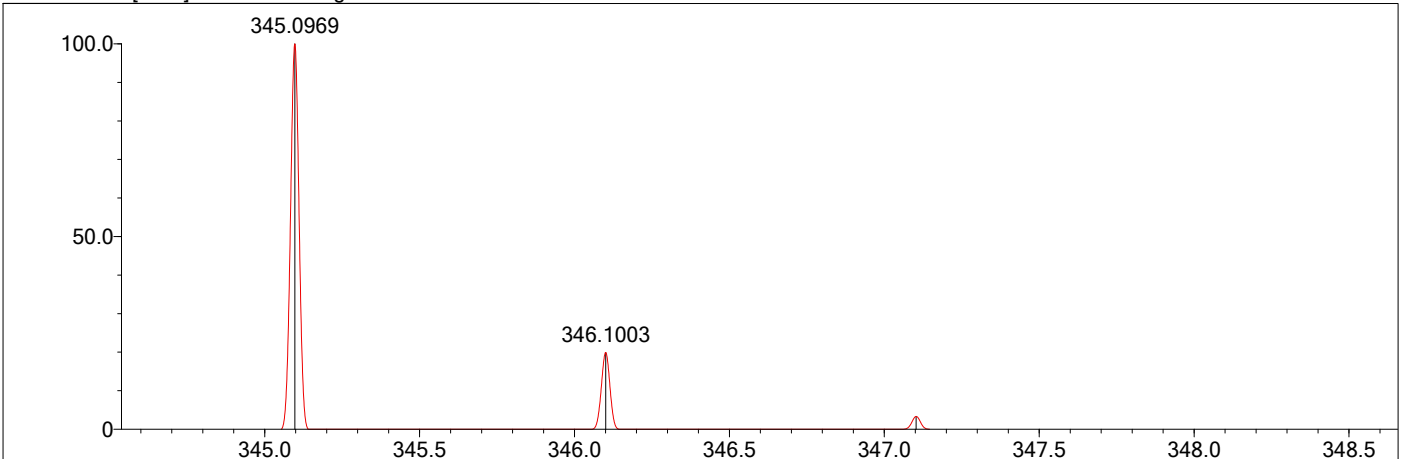
2j



Measured region for 345.0961 m/z



C18 H16 O7 [M+H]+ : Predicted region for 345.0969 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	64.41	C18 H16 O7	[M+H]+	345.0961	345.0969	-0.8	-2.32	66.60	11.0

Data File: F:\高分辨数据\Zouyong\SXH\SJF-2K.Icd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	12	O	2	0	3	Cl	1	0	0	H
B	3	0	0	F	1	0	0	Br	1	0	0	Na
C	4	0	16	P	3	0	0	I	3	0	0	K
N	3	0	0	S	2	0	0					NH4

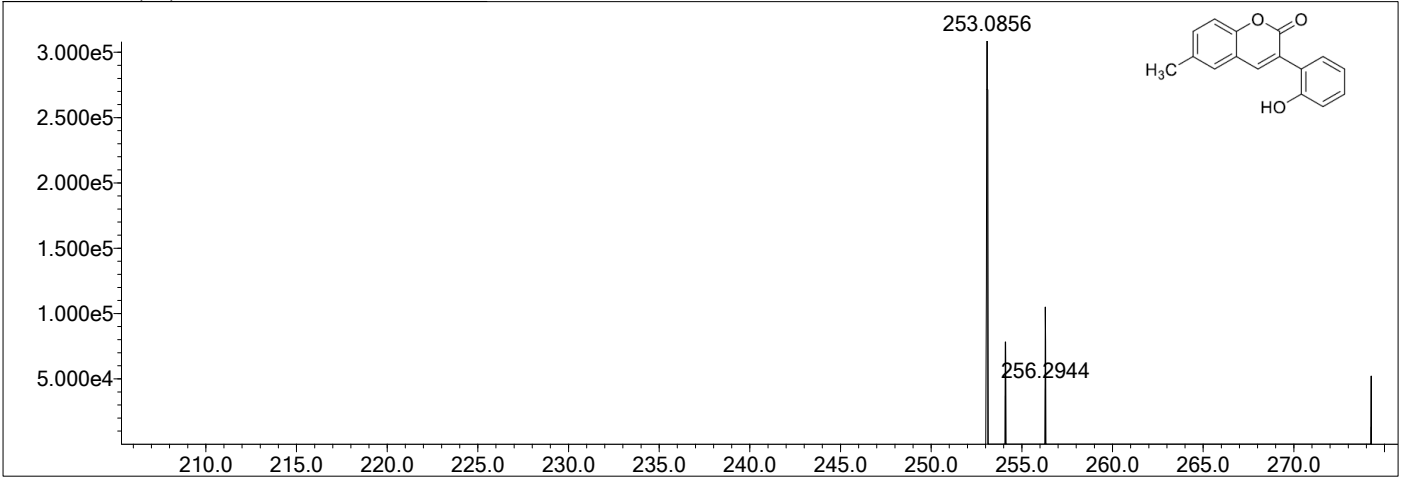
Error Margin (ppm): 5  
 HC Ratio: unlimited  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

DBE Range: -1.0 - 1500.0  
 Apply N Rule: no  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

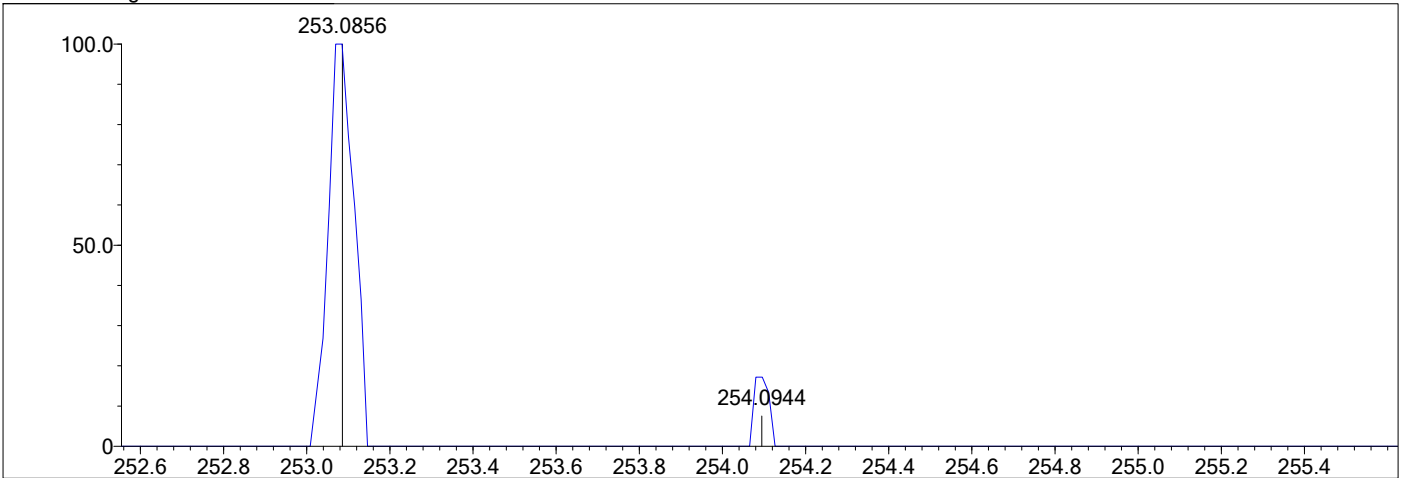
Electron Ions: both  
 Use MSn Info: no  
 Isotope Res: 10000  
 Max Results: 40

Event#: 1 MS(E+) Ret. Time : 0.853 Scan#: 129

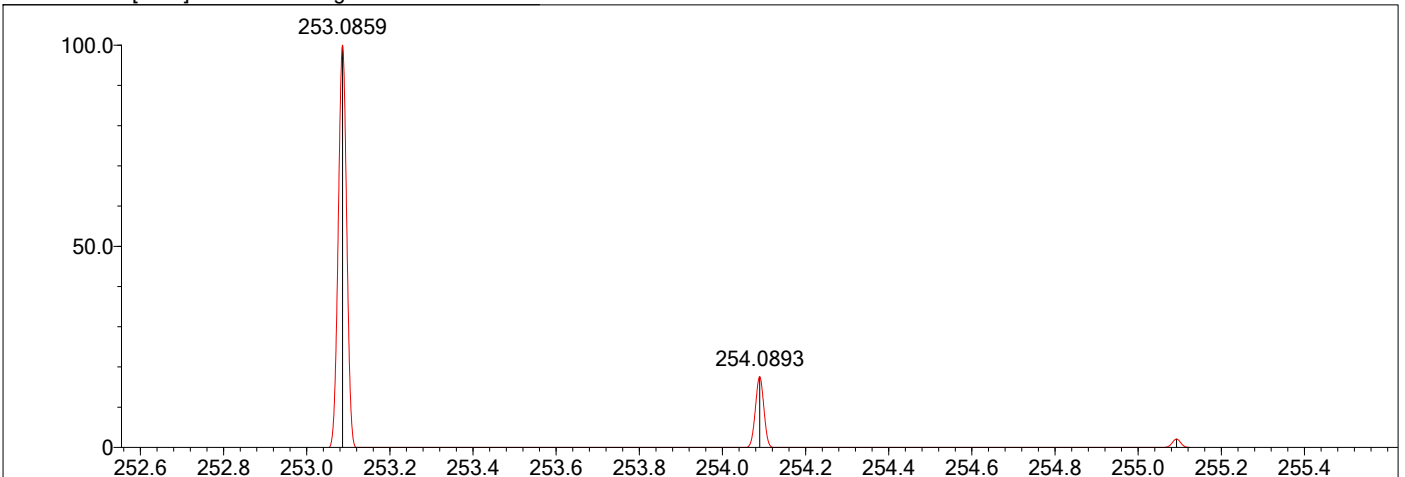
2k



Measured region for 253.0856 m/z



C16 H12 O3 [M+H]<sup>+</sup> : Predicted region for 253.0859 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	73.36	C16 H12 O3	[M+H] <sup>+</sup>	253.0856	253.0859	-0.3	-1.19	73.71	11.0

Data File: F:\高分辨数据\Zouyong\SXH\SJF-2L.lcd

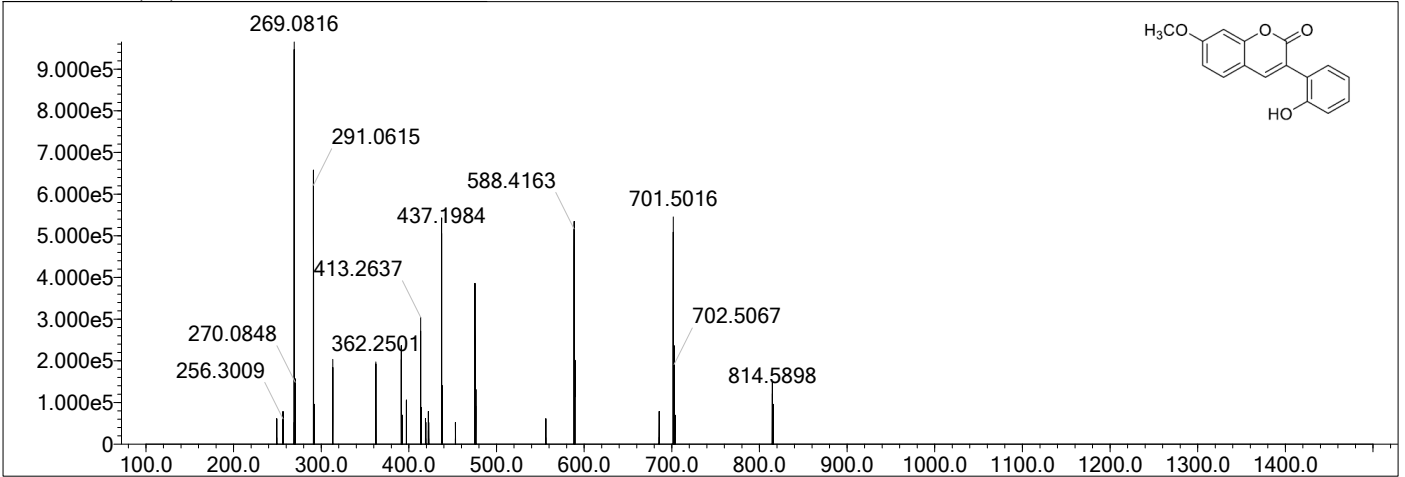
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	12	O	2	0	4	Cl	1	0	0	H
B	3	0	0	F	1	0	0	Br	1	0	0	Na
C	4	0	16	P	3	0	0	I	3	0	0	K
N	3	0	0	S	2	0	0					NH4

Error Margin (ppm): 5  
 HC Ratio: unlimited  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

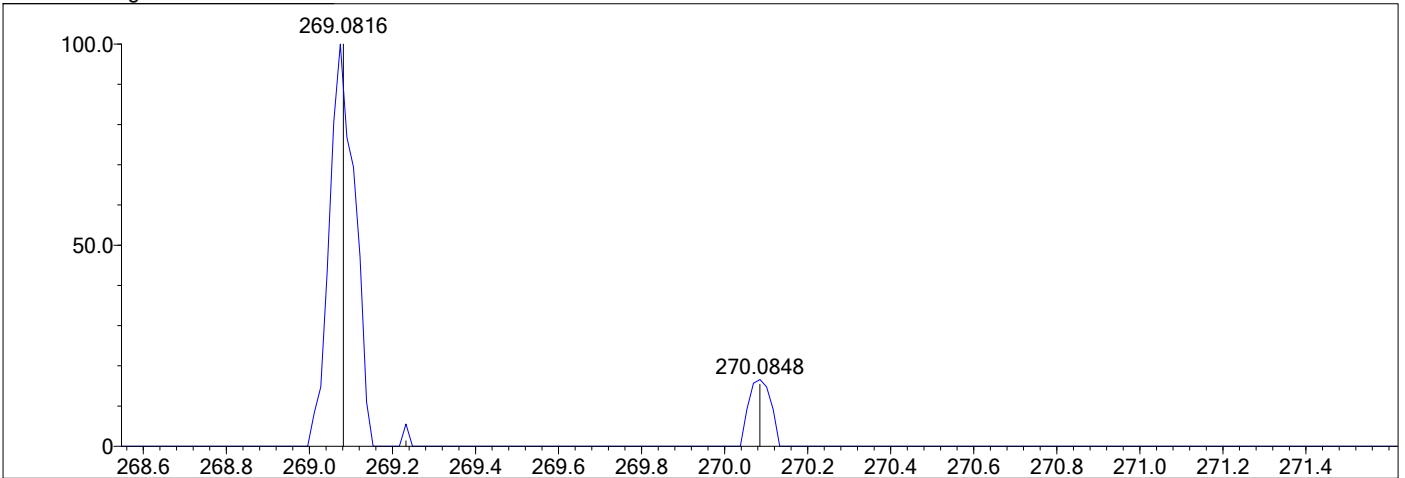
DBE Range: -1.0 - 1500.0  
 Apply N Rule: no  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

Electron Ions: both  
 Use MSn Info: no  
 Isotope Res: 10000  
 Max Results: 40

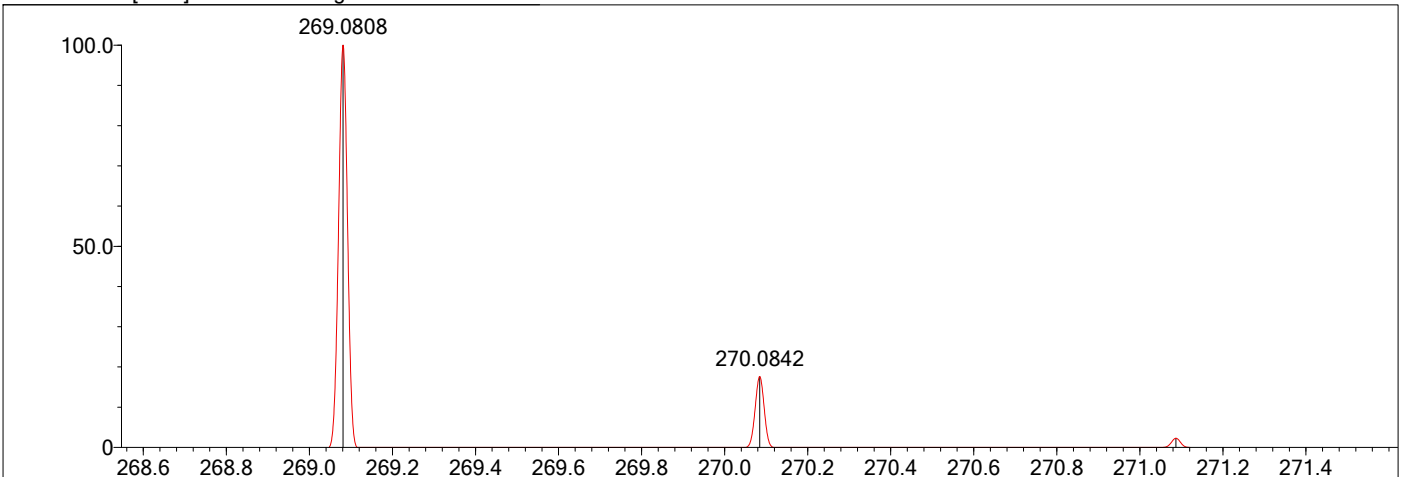
Event#: 1 MS(E+) Ret. Time : 0.840 Scan# : 127



Measured region for 269.0816 m/z



C16 H12 O4 [M+H]<sup>+</sup> : Predicted region for 269.0808 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	48.37	C16 H12 O4	[M+H] <sup>+</sup>	269.0816	269.0808	0.8	2.97	50.87	11.0

Data File: F:\高分辨数据\Zouyong\SXH\SJF-2M.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	9	O	2	0	3	Cl	1	0	1	H
B	3	0	0	F	1	0	0	Br	1	0	0	HCOO
C	4	0	15	P	3	0	0	I	3	0	0	CH3COO
N	3	0	0	S	2	0	0					Cl

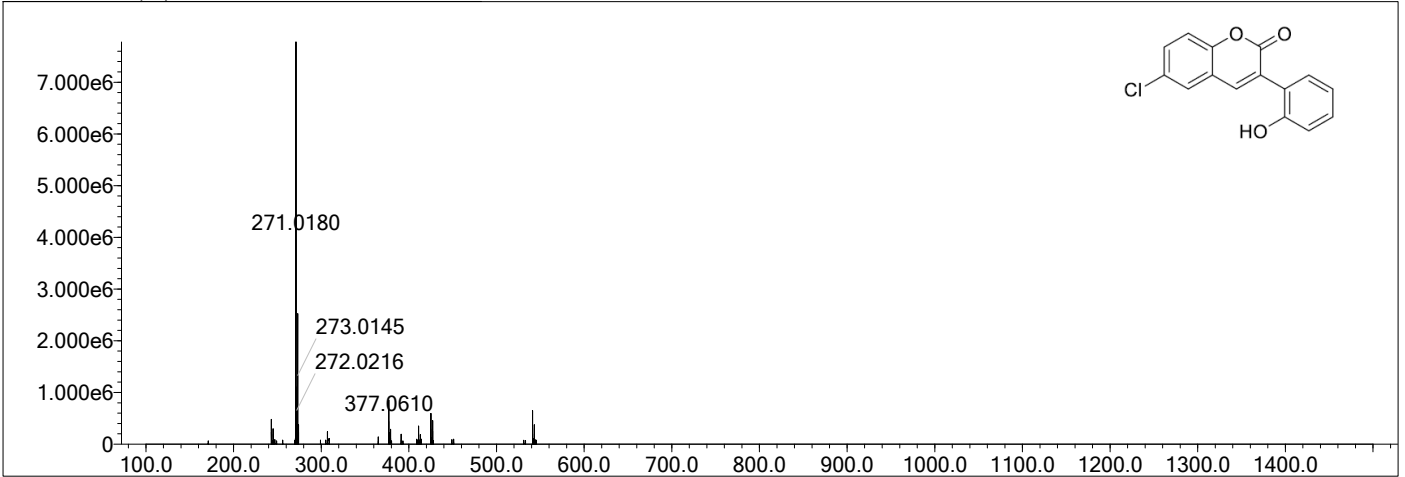
Error Margin (ppm): 5  
 HC Ratio: unlimited  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

DBE Range: -1.0 - 1500.0  
 Apply N Rule: no  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

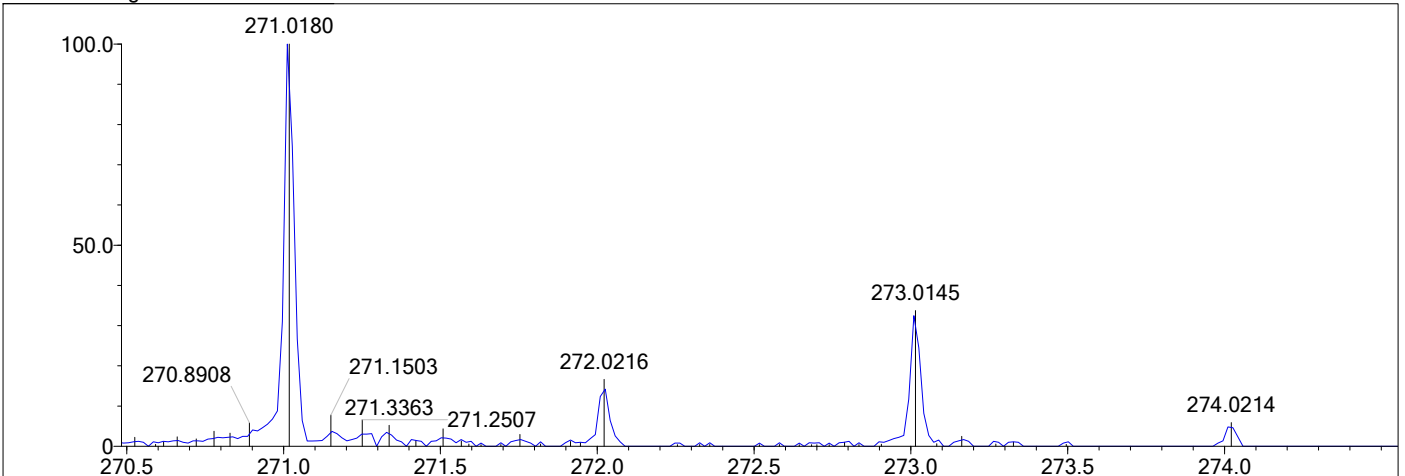
Electron Ions: both  
 Use MSn Info: no  
 Isotope Res: 10000  
 Max Results: 40

Event#: 2 MS(E-) Ret. Time : 0.987 Scan#: 150

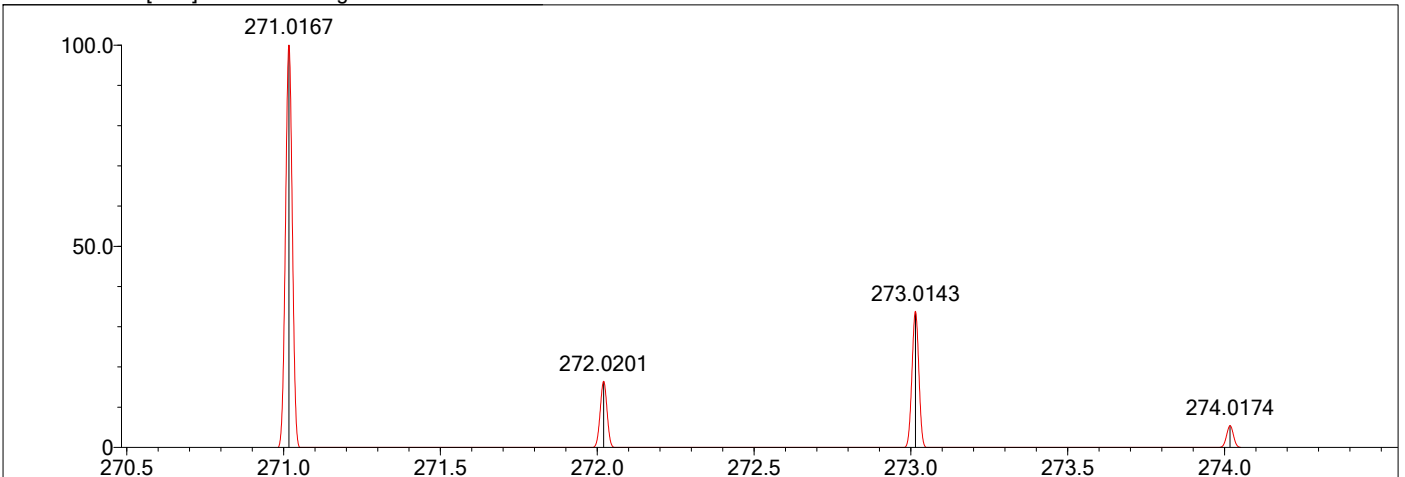
2m



Measured region for 271.0180 m/z



C15 H9 O3 Cl [M-H]-: Predicted region for 271.0167 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	64.06	C15 H9 O3 Cl	[M-H]-	271.0180	271.0167	1.3	4.80	70.78	11.0

Data File: \\Deep-20160624\data1\邹永\SXH\SJF-2N.Icd

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	7	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	K
B	3	0	0	P	3	0	0	Cu	2	0	0	Au	1	0	0	
C	4	0	30	S	2	0	0	Se	2	0	0					
N	3	0	8	Cl	1	0	0	Br	1	0	0					

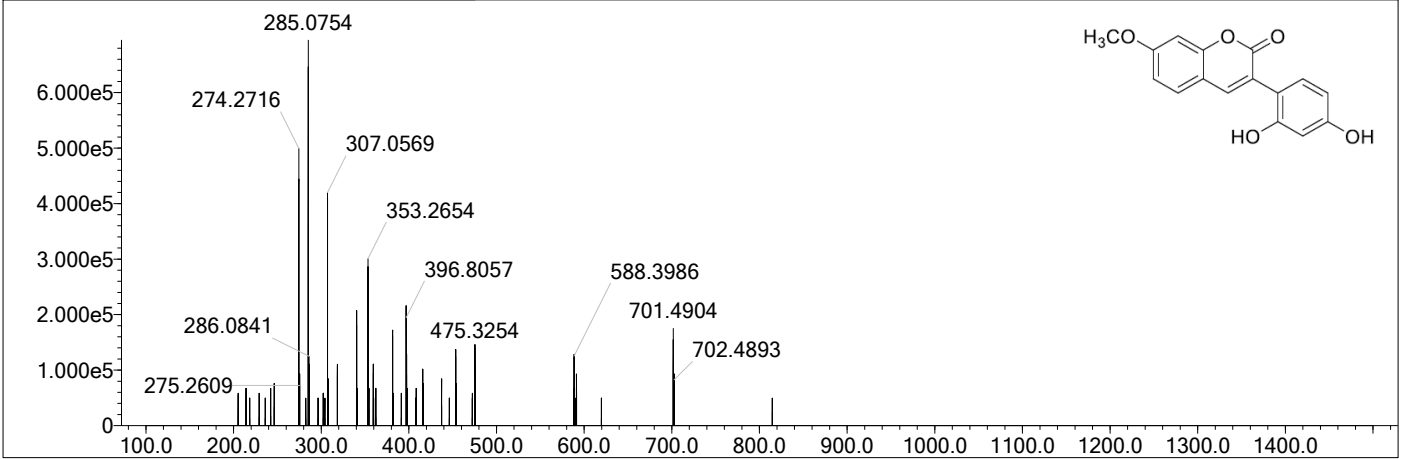
Error Margin (ppm): 50  
 HC Ratio: 0.0 - 20.0  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

DBE Range: -100.0 - 1000.0  
 Apply N Rule: yes  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

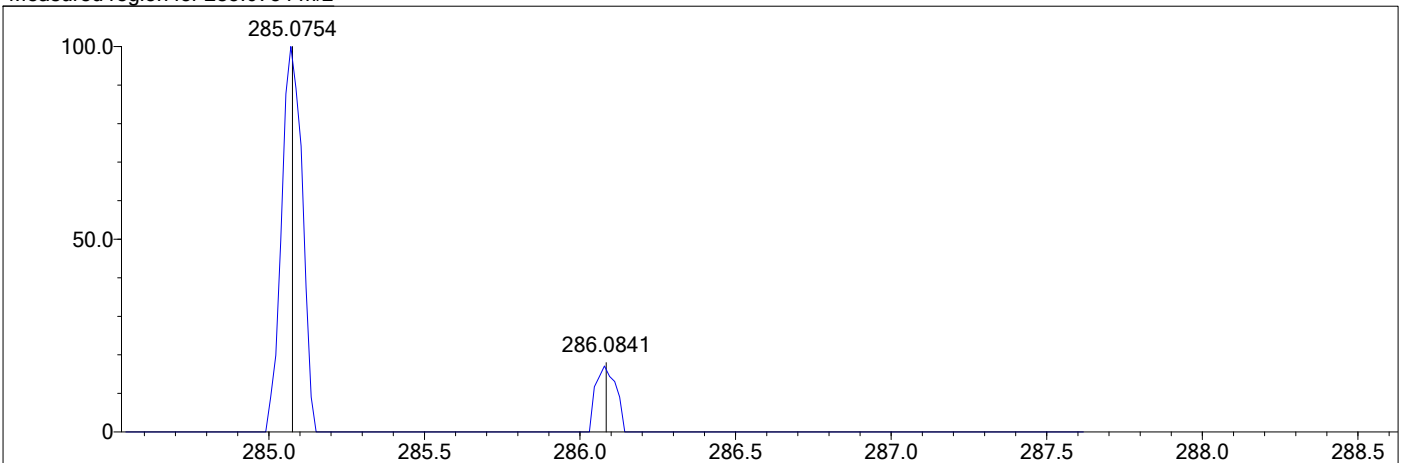
Electron Ions: both  
 Use MSn Info: no  
 Isotope Res: 10000  
 Max Results: 2000

Event#: 1 MS(E+) Ret. Time : 0.147 Scan#: 23

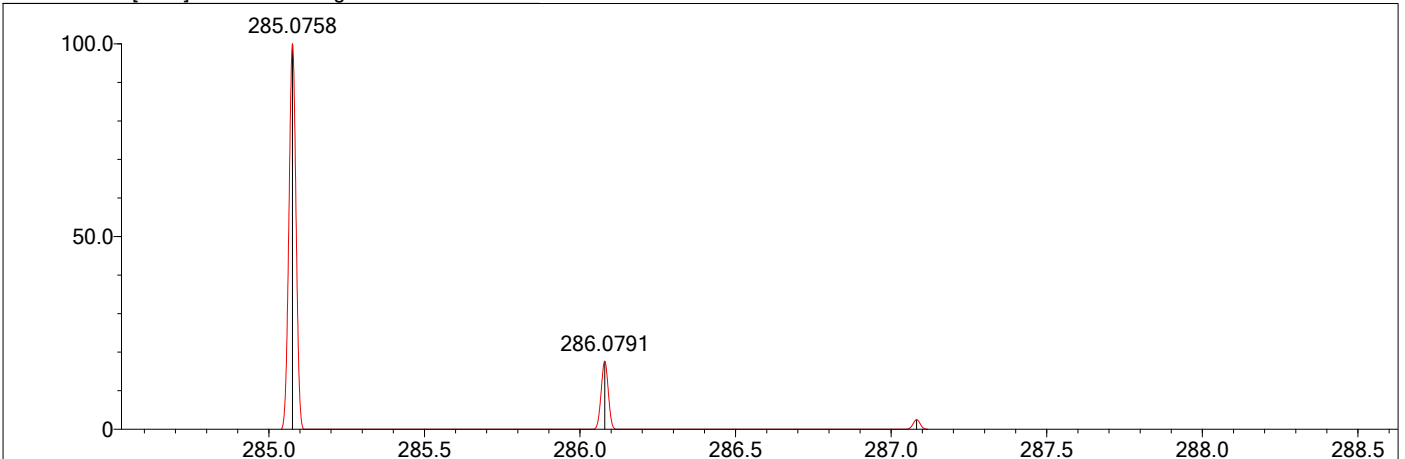
2n



Measured region for 285.0754 m/z



C16 H12 O5 [M+H]+ : Predicted region for 285.0758 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	72.21	C16 H12 O5	[M+H]+	285.0754	285.0758	-0.4	-1.40	72.94	11.0

Data File: \\Deep-20160624\l\data1\邹永\SXH\SJF-2O.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	7	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	K
B	3	0	0	P	3	0	0	Cu	2	0	0	Au	1	0	0	
C	4	0	30	S	2	0	0	Se	2	0	0					
N	3	0	8	Cl	1	0	0	Br	1	0	0					

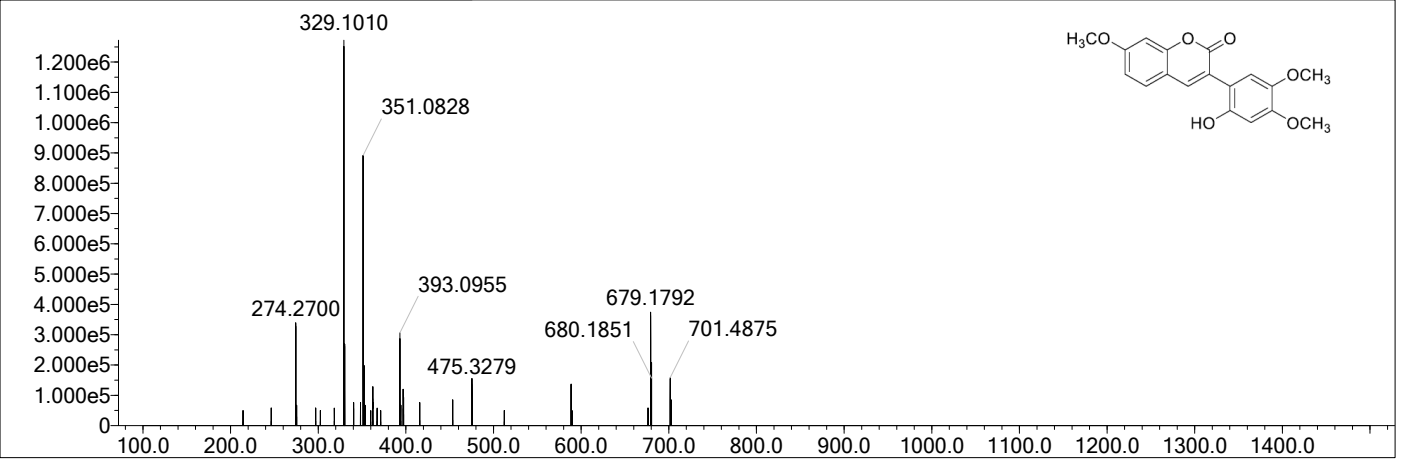
Error Margin (ppm): 50  
 HC Ratio: 0.0 - 20.0  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

DBE Range: -100.0 - 1000.0  
 Apply N Rule: yes  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

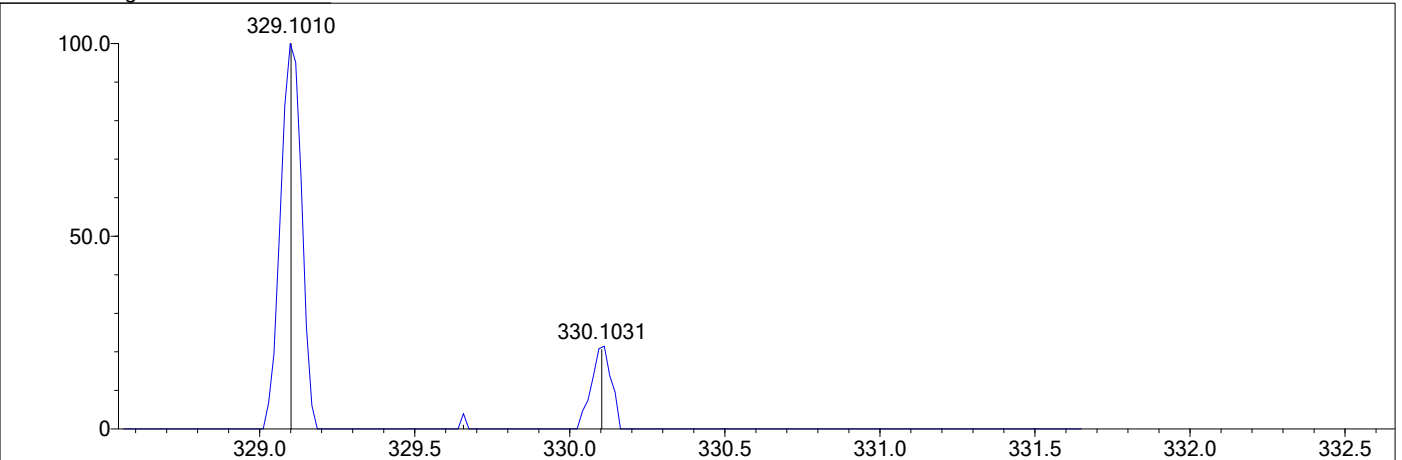
Electron Ions: both  
 Use MSn Info: no  
 Isotope Res: 10000  
 Max Results: 2000

Event#: 1 MS(E+) Ret. Time : 0.160 Scan#: 25

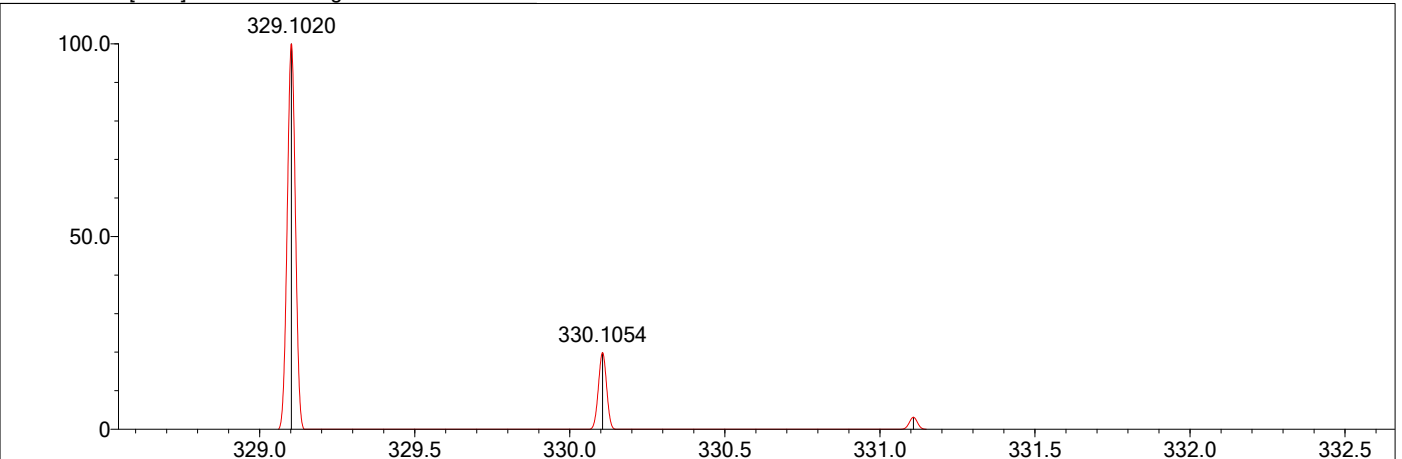
20



Measured region for 329.1010 m/z



C18 H16 O6 [M+H]<sup>+</sup> : Predicted region for 329.1020 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	82.23	C18 H16 O6	[M+H] <sup>+</sup>	329.1010	329.1020	-1.0	-3.04	86.65	11.0

Data File: \\Deep-20160624\data1\邹永\SXH\SJF-2P.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	7	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	K
B	3	0	0	P	3	0	0	Cu	2	0	0	Au	1	0	0	
C	4	0	30	S	2	0	0	Se	2	0	0					
N	3	0	8	Cl	1	0	0	Br	1	0	0					

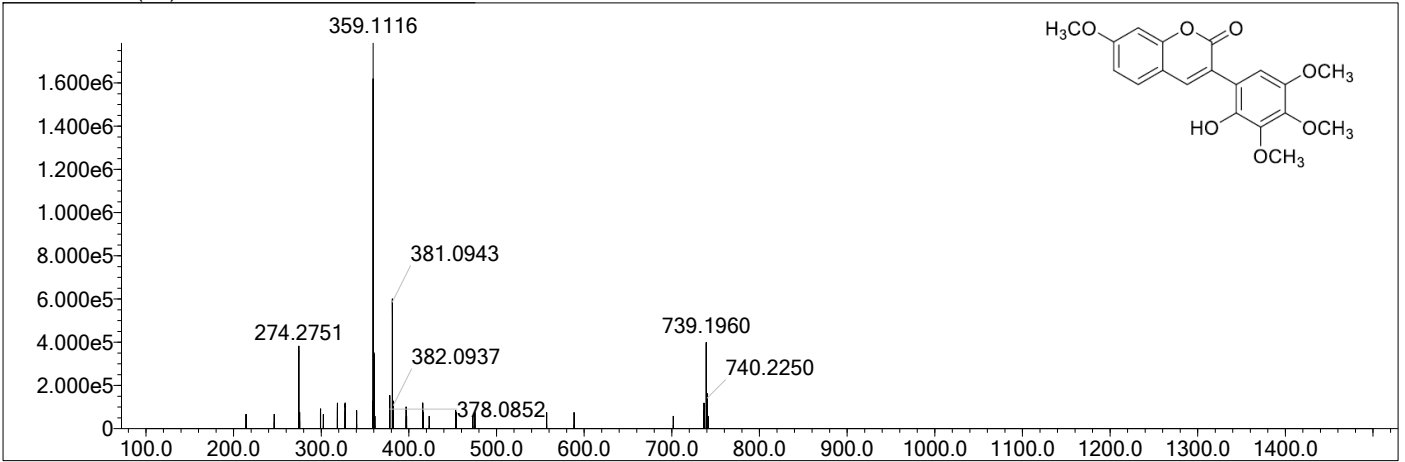
Error Margin (ppm): 50  
 HC Ratio: 0.0 - 20.0  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

DBE Range: -100.0 - 1000.0  
 Apply N Rule: yes  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

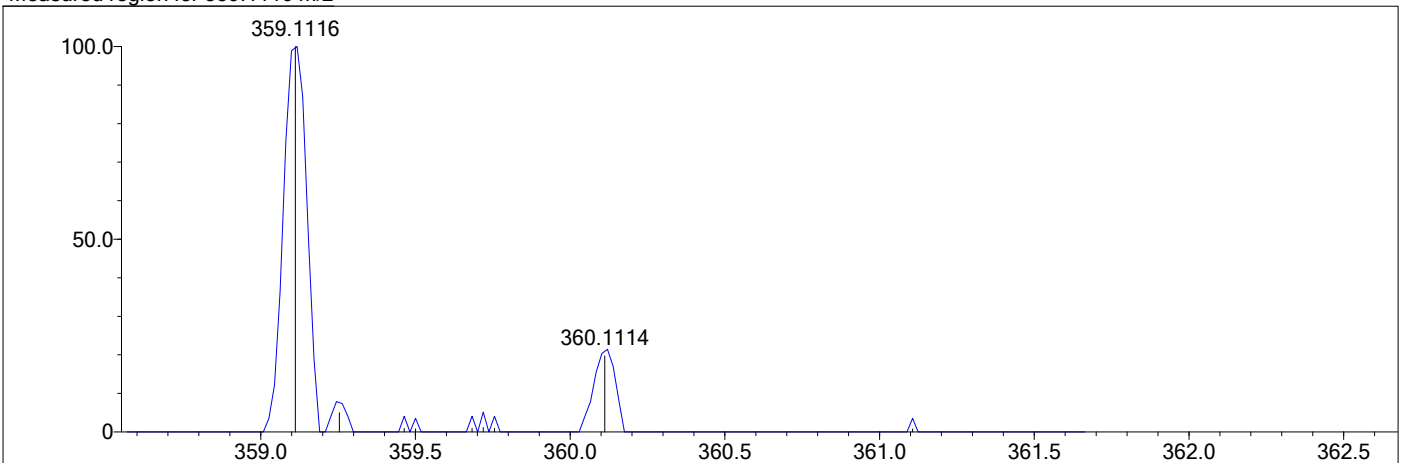
Electron Ions: both  
 Use MSn Info: no  
 Isotope Res: 10000  
 Max Results: 2000

Event#: 1 MS(E+) Ret. Time : 0.147 Scan# : 23

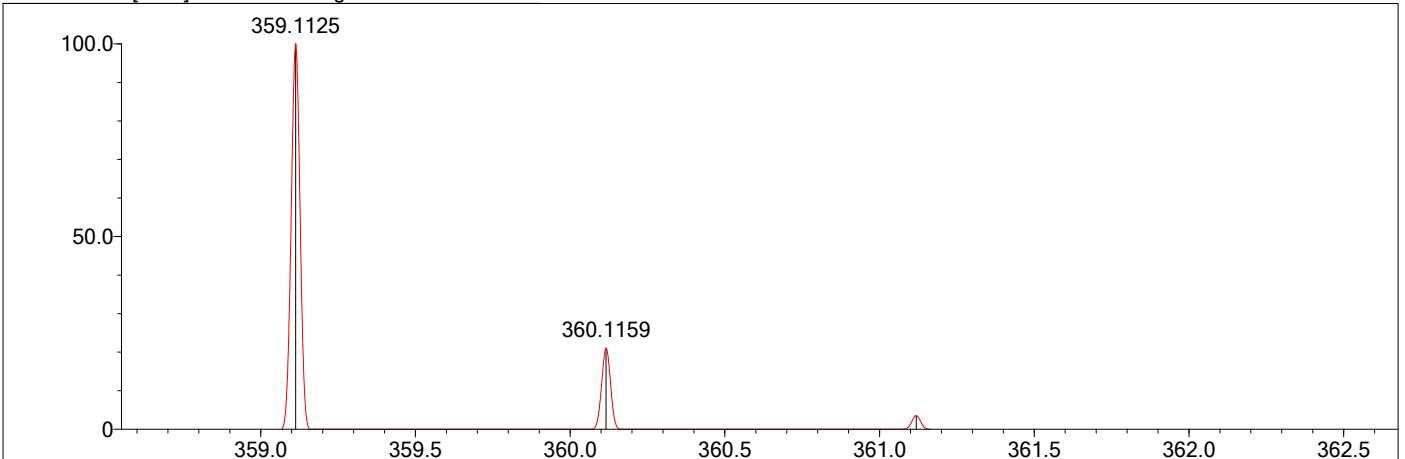
2p



Measured region for 359.1116 m/z



C19 H18 O7 [M+H]<sup>+</sup> : Predicted region for 359.1125 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
4	61.78	C19 H18 O7	[M+H] <sup>+</sup>	359.1116	359.1125	-0.9	-2.51	64.20	11.0



Data File: \\Deep-20160624\l\data1\邹永\SXH\SJF-2Q.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	7	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	K
B	3	0	0	P	3	0	0	Cu	2	0	0	Au	1	0	0	
C	4	0	30	S	2	0	0	Se	2	0	0					
N	3	0	8	Cl	1	0	0	Br	1	0	0					

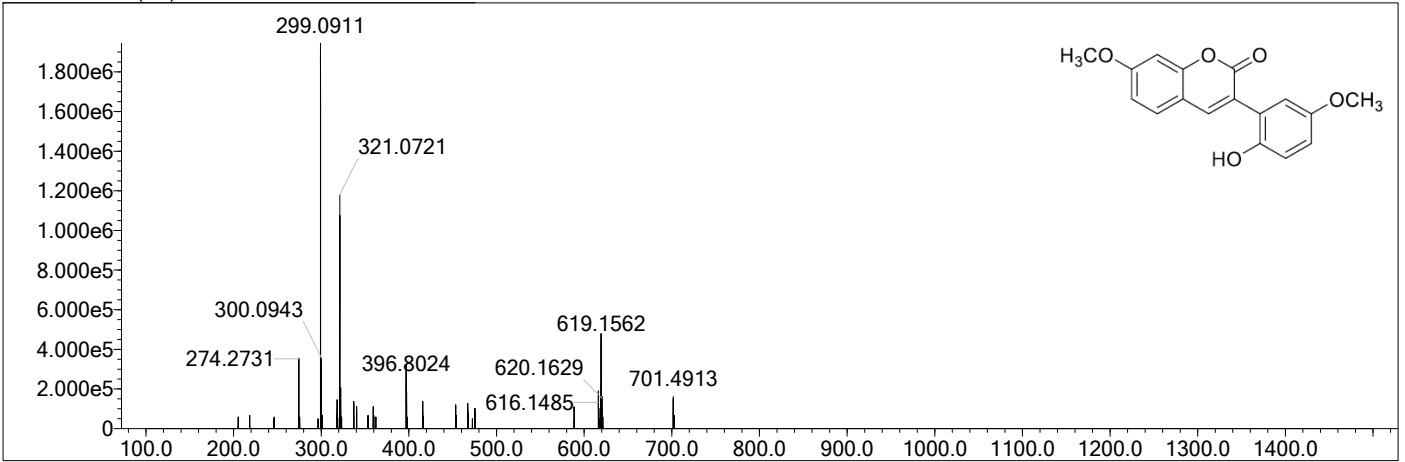
Error Margin (ppm): 50  
 HC Ratio: 0.0 - 20.0  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

DBE Range: -100.0 - 1000.0  
 Apply N Rule: yes  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

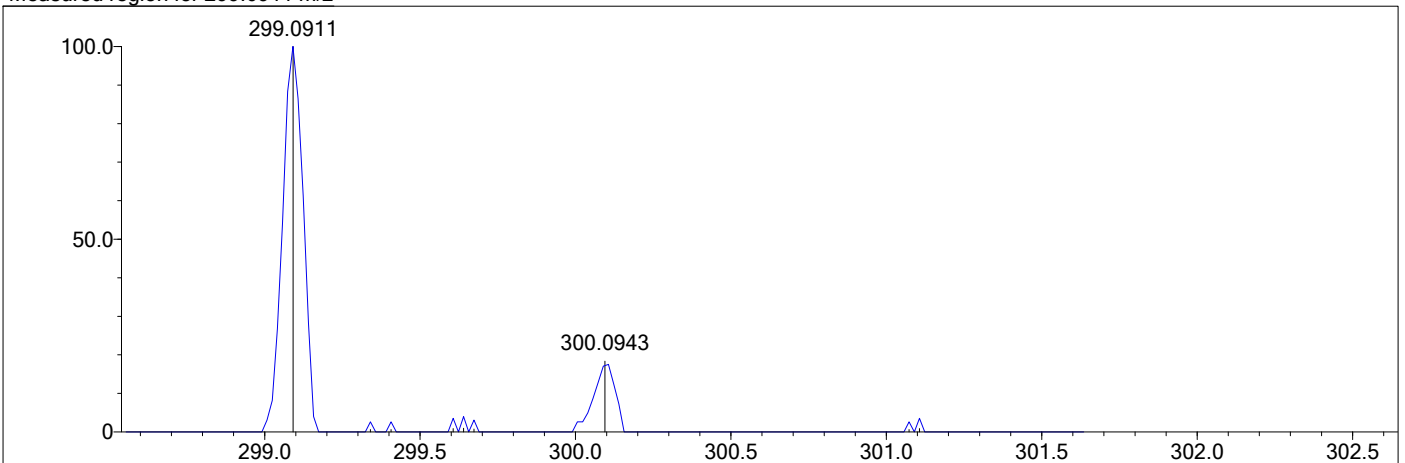
Electron Ions: both  
 Use MSn Info: no  
 Isotope Res: 10000  
 Max Results: 2000

Event#: 1 MS(E+) Ret. Time: 0.160 Scan#: 25

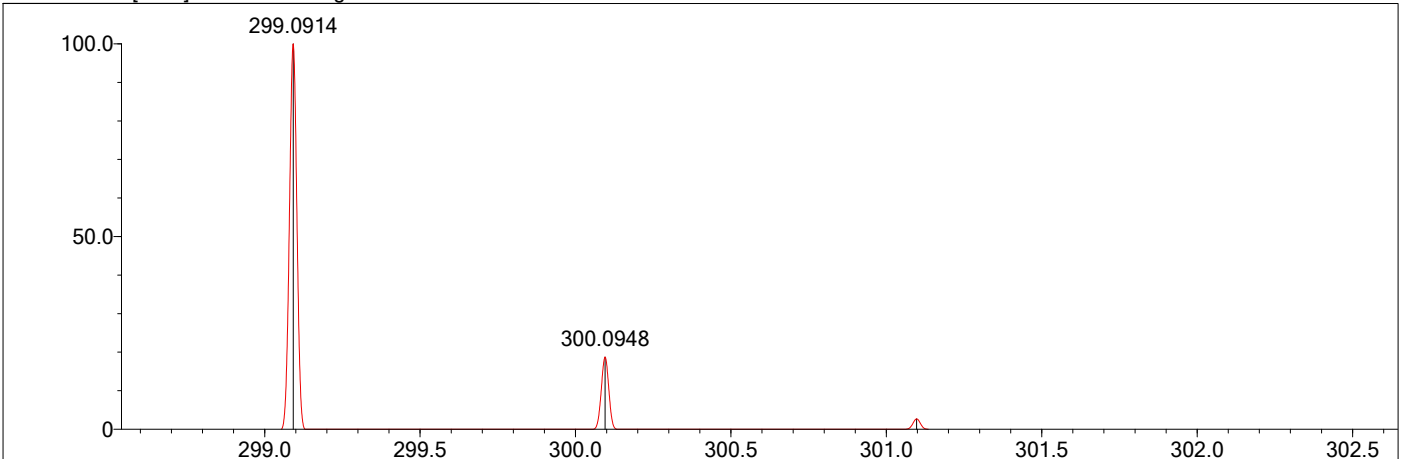
2q



Measured region for 299.0911 m/z



C17 H14 O5 [M+H]+ : Predicted region for 299.0914 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	78.60	C17 H14 O5	[M+H] <sup>+</sup>	299.0911	299.0914	-0.3	-1.00	78.60	11.0

Data File: F:\高分辨数据\Zouyong\SXH\SJF-2R.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	18	O	2	0	7	Cl	1	0	0	H
B	3	0	0	F	1	0	0	Br	1	0	0	Na
C	4	0	19	P	3	0	0	I	3	0	0	K
N	3	0	0	S	2	0	0					NH4

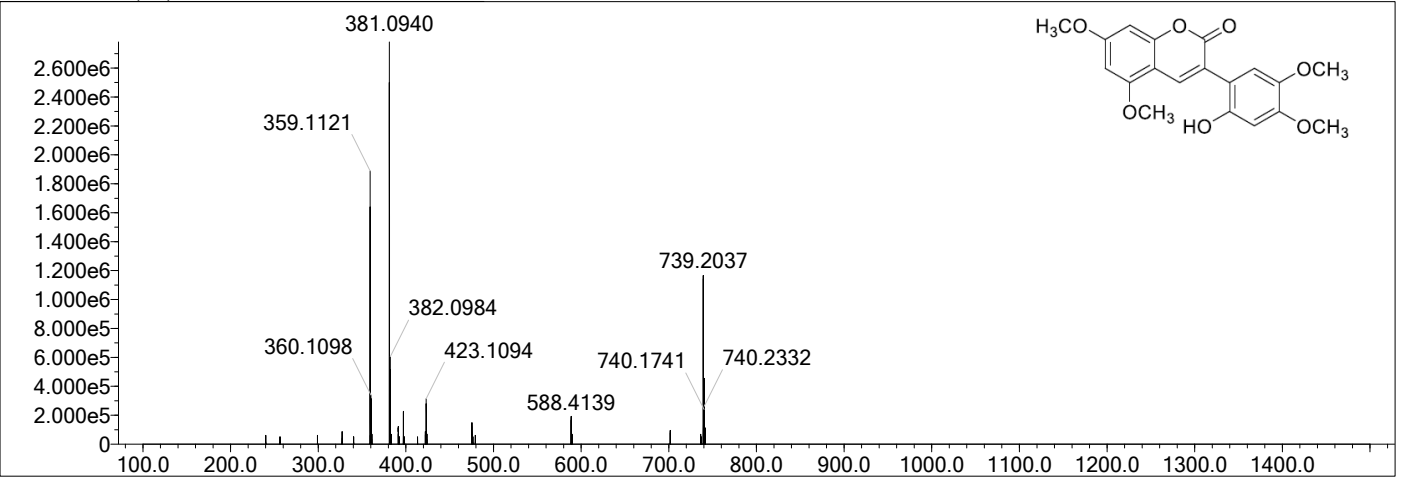
Error Margin (ppm): 5  
 HC Ratio: unlimited  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

DBE Range: -1.0 - 1500.0  
 Apply N Rule: no  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

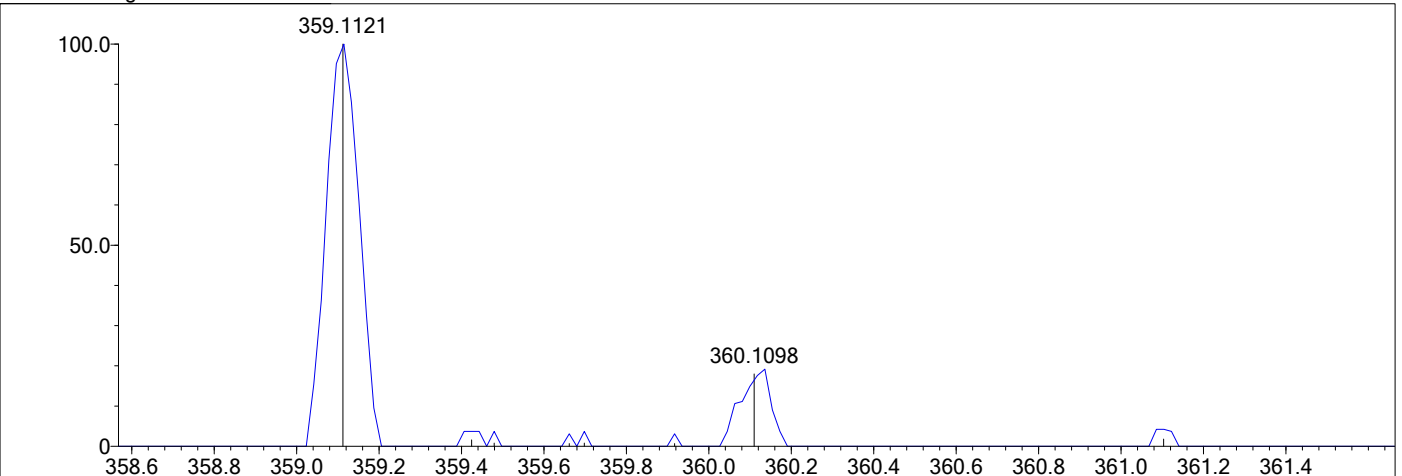
Electron Ions: both  
 Use MSn Info: no  
 Isotope Res: 10000  
 Max Results: 40

Event#: 1 MS(E+) Ret. Time: 0.893 Scan#: 135

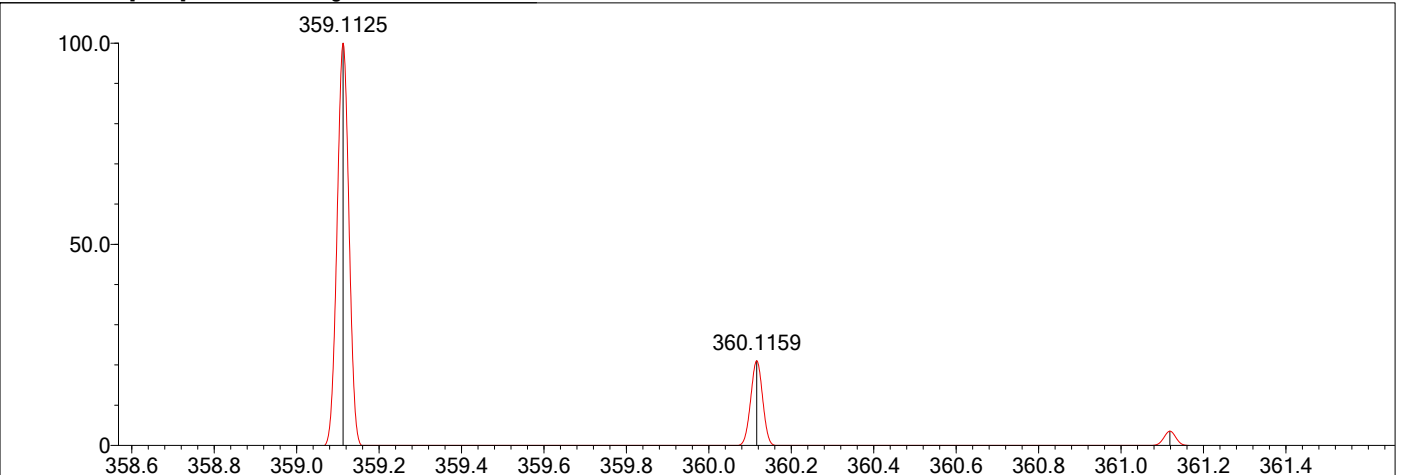
2r



Measured region for 359.1121 m/z



C19H18O7 [M+H]<sup>+</sup> : Predicted region for 359.1125 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	63.36	C19H18O7	[M+H] <sup>+</sup>	359.1121	359.1125	-0.4	-1.11	63.53	11.0

Data File: \\Deep-20160624\data1\邹永\SXH\SJF-2S.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	8	10	O	2	3	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	
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	15	15	S	2	0	0	Se	2	0	0					
N	3	0	0	Cl	1	0	0	Br	1	0	0					

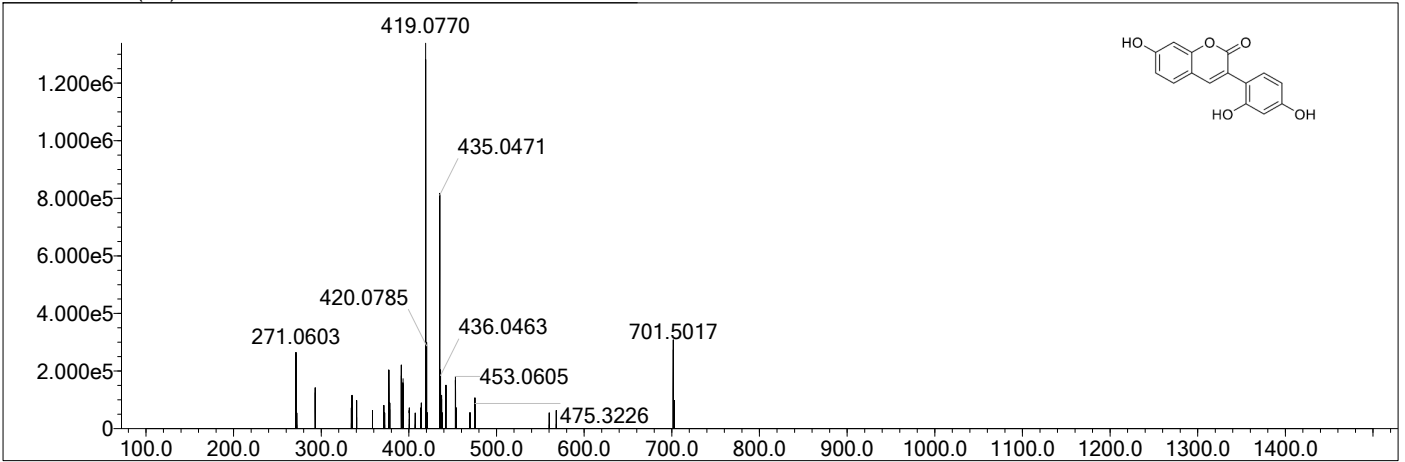
Error Margin (ppm): 100  
 HC Ratio: 0.0 - 100.0  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

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

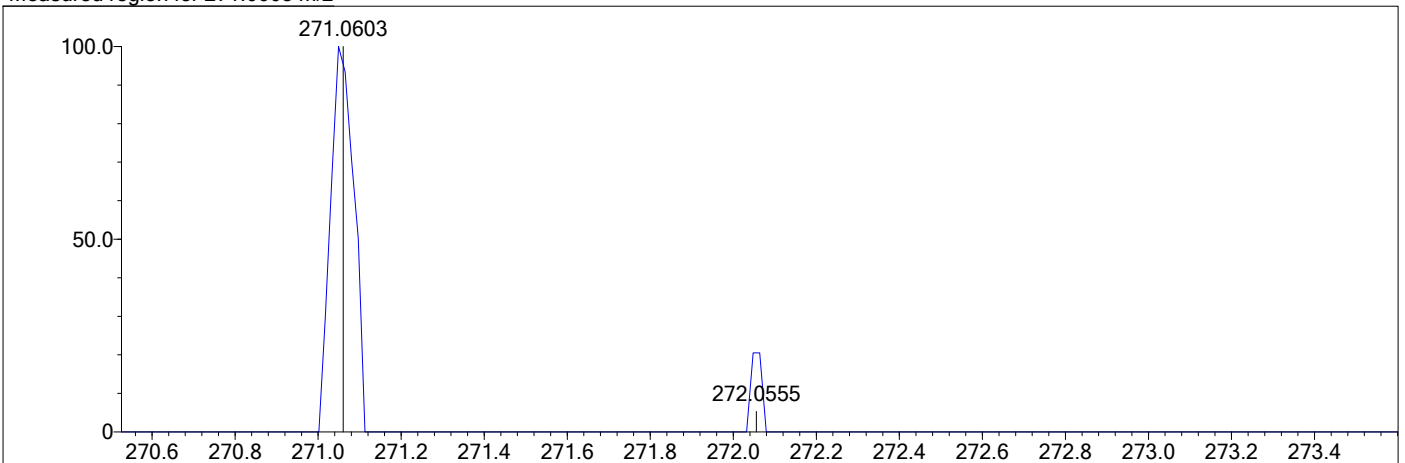
Electron Ions: both  
 Use MSn Info: no  
 Isotope Res: 10000  
 Max Results: 100

Event#: 1 MS(E+) Ret. Time : 0.827 -> 0.827 Scan# : 125 -> 125

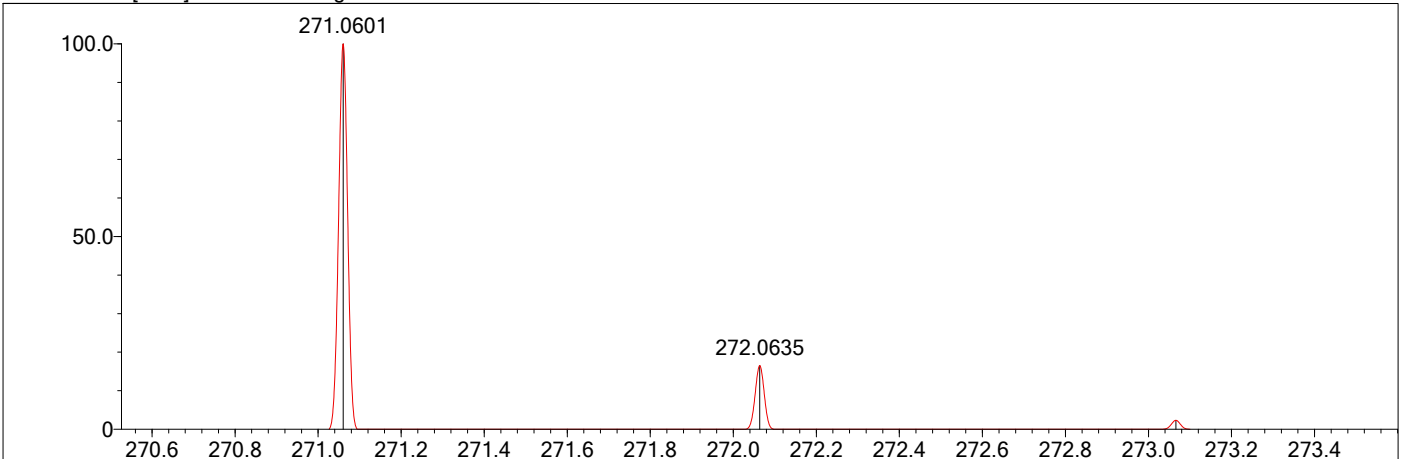
2s



Measured region for 271.0603 m/z



C15 H10 O5 [M+H]+ : Predicted region for 271.0601 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	44.53	C15 H10 O5	[M+H]+	271.0603	271.0601	0.2	0.74	44.53	11.0

Data File: F:\高分辨数据\Zouyong\SXH\SJF-2T.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	12	O	2	0	5	Cl	1	0	0	H
B	3	0	0	F	1	0	0	Br	1	0	0	Na
C	4	0	16	P	3	0	0	I	3	0	0	K
N	3	0	0	S	2	0	0					NH4

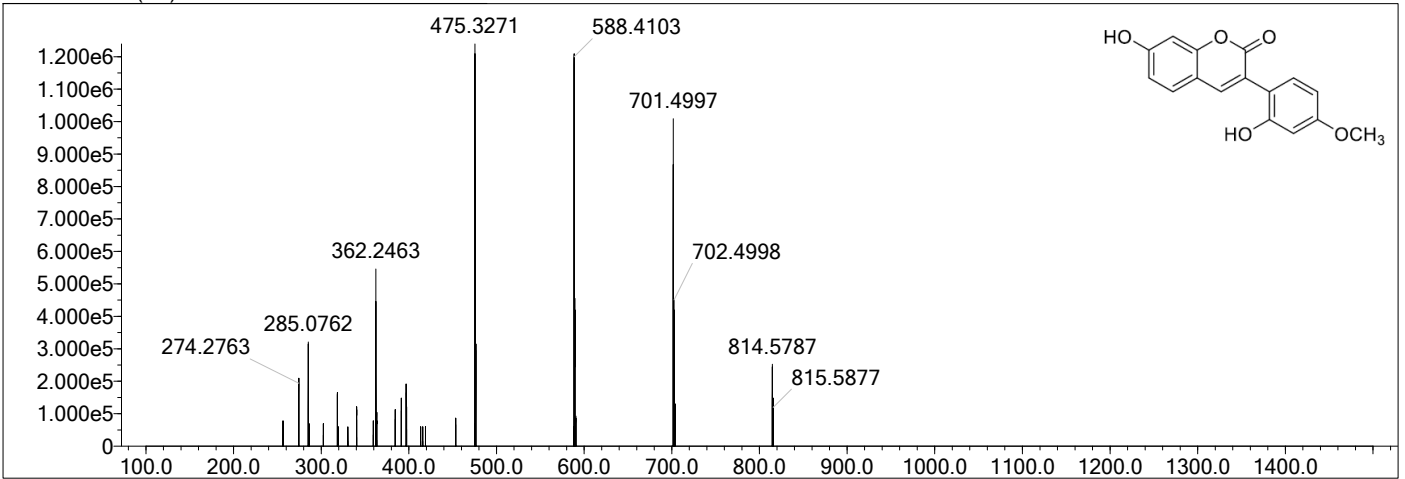
Error Margin (ppm): 5  
 HC Ratio: unlimited  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

DBE Range: -1.0 - 1500.0  
 Apply N Rule: no  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

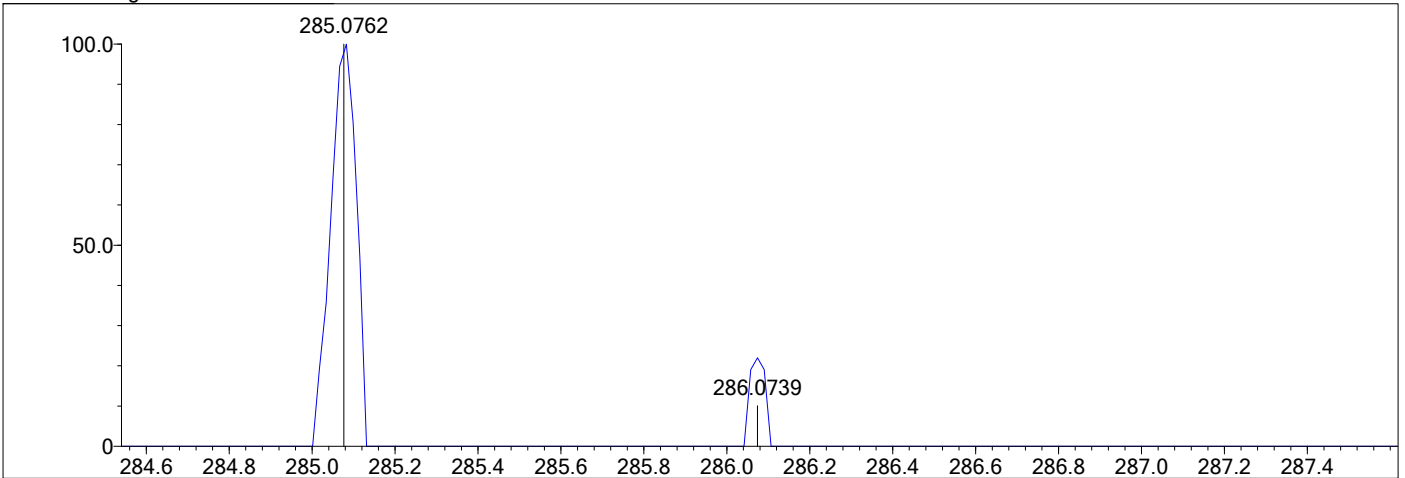
Electron Ions: both  
 Use MSn Info: no  
 Isotope Res: 10000  
 Max Results: 40

Event#: 1 MS(E+) Ret. Time : 0.693 Scan# : 105

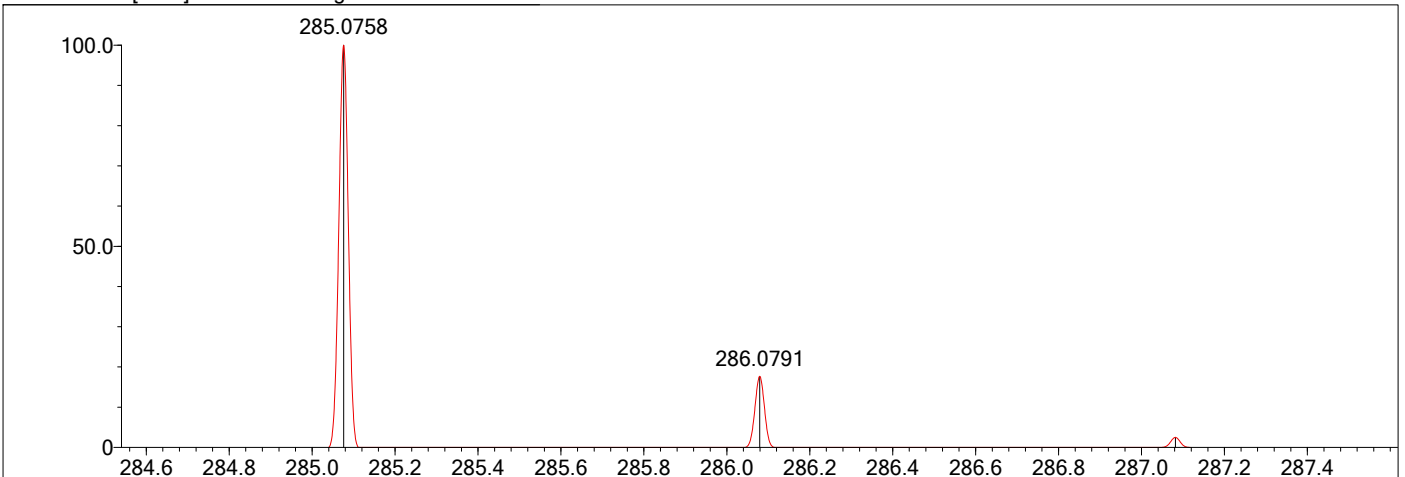
2t



Measured region for 285.0762 m/z



C16 H12 O5 [M+H]<sup>+</sup> : Predicted region for 285.0758 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	64.35	C16 H12 O5	[M+H] <sup>+</sup>	285.0762	285.0758	0.4	1.40	65.00	11.0

Data File: F:\高分辨数据\Zouyong\SXH\SJF-2U.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	14	O	2	0	6	Cl	1	0	0	H
B	3	0	0	F	1	0	0	Br	1	0	0	Na
C	4	0	17	P	3	0	0	I	3	0	0	K
N	3	0	0	S	2	0	0					NH4

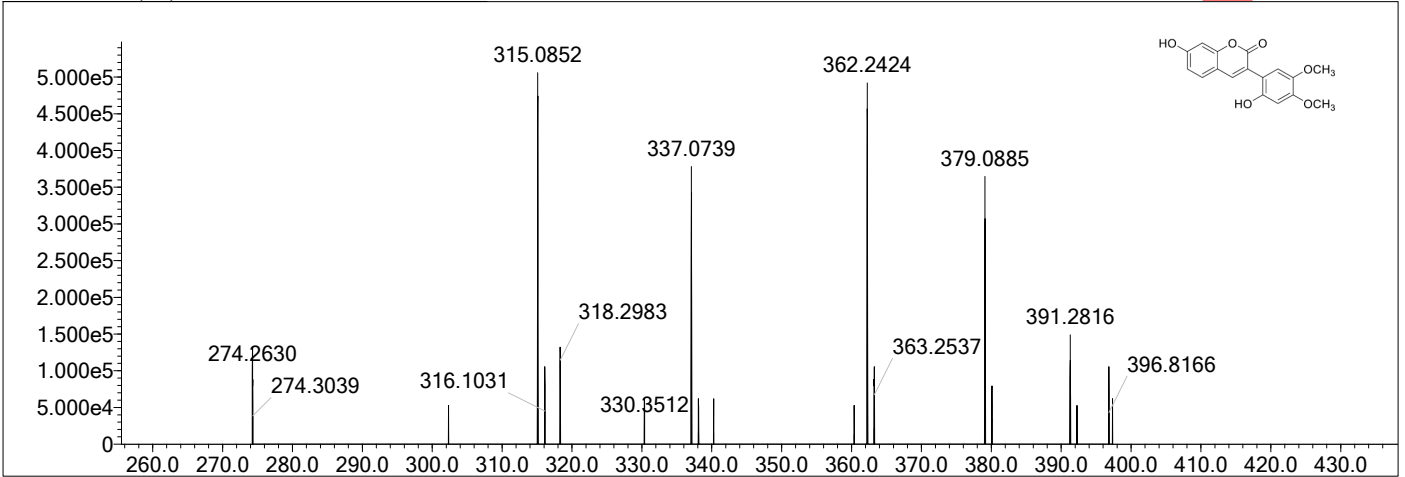
Error Margin (ppm): 5  
 HC Ratio: unlimited  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

DBE Range: -1.0 - 1500.0  
 Apply N Rule: no  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

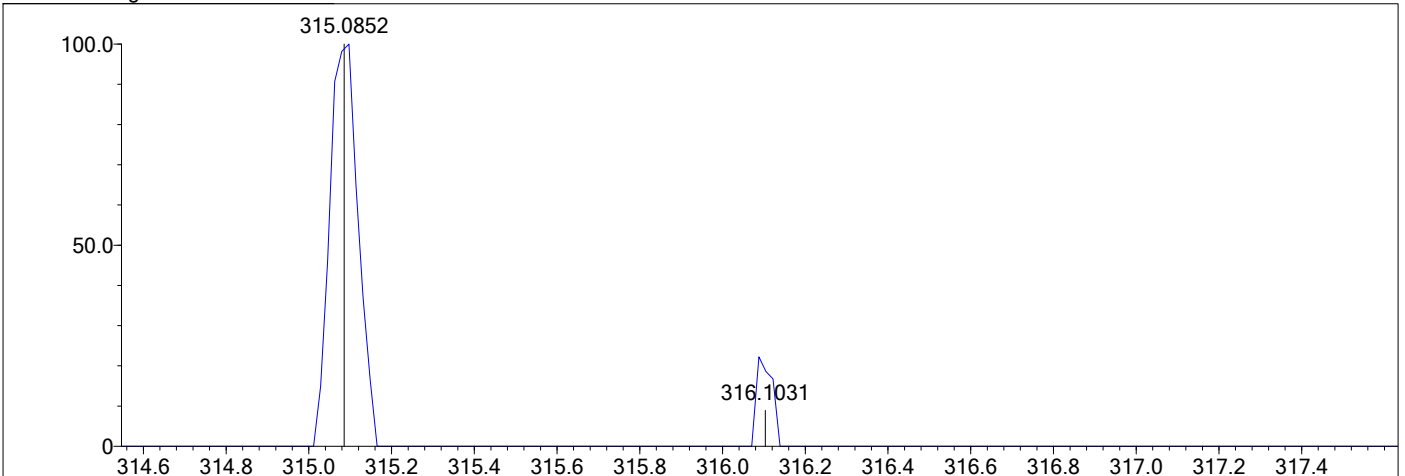
Electron Ions: both  
 Use MSn Info: no  
 Isotope Res: 10000  
 Max Results: 40

Event#: 1 MS(E+) Ret. Time : 0.707 Scan#: 107

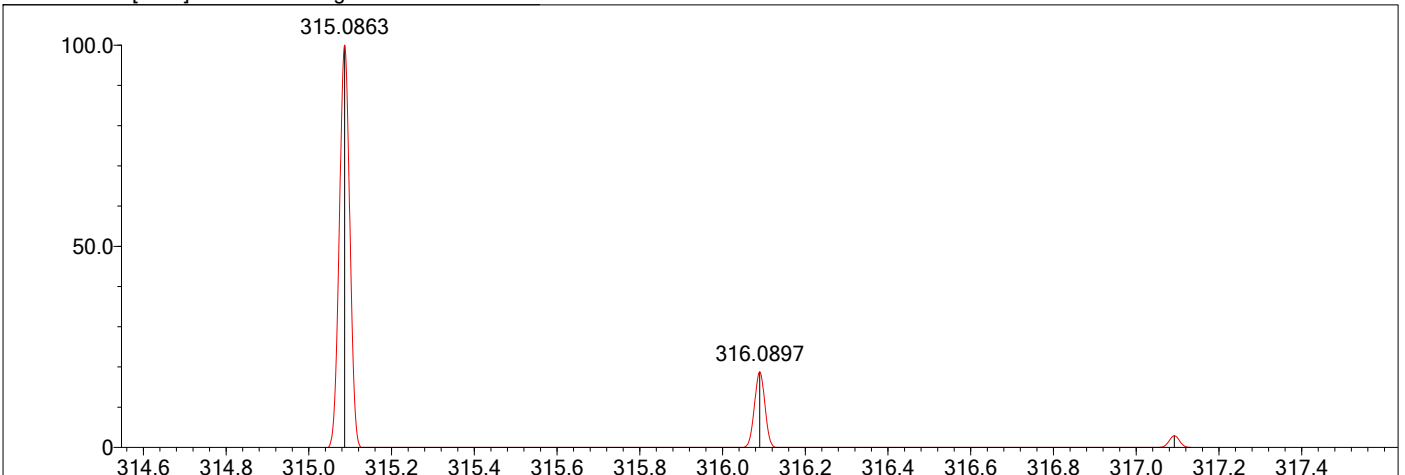
2u



Measured region for 315.0852 m/z



C17 H14 O6 [M+H]+ : Predicted region for 315.0863 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	52.70	C17 H14 O6	[M+H]+	315.0852	315.0863	-1.1	-3.49	56.20	11.0

Data File: F:\高分辨数据\Zouyong\SXH\SJF-2V.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	10	O	2	0	6	Cl	1	0	0	H
B	3	0	0	F	1	0	0	Br	1	0	0	HCOO
C	4	0	16	P	3	0	0	I	3	0	0	CH3COO
N	3	0	0	S	2	0	0					Cl

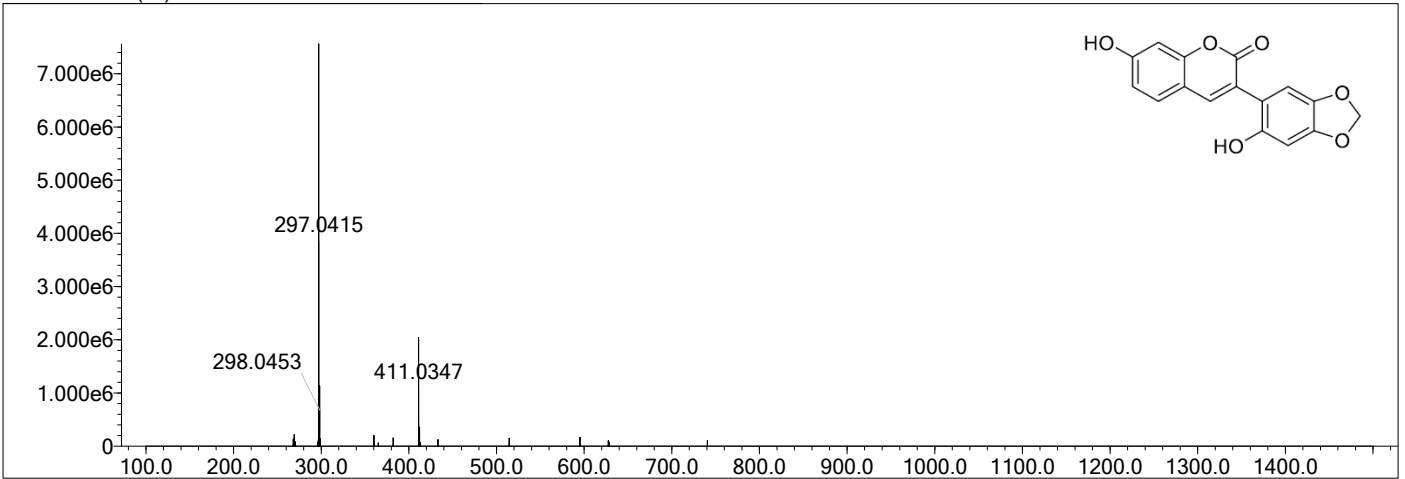
Error Margin (ppm): 5  
 HC Ratio: unlimited  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

DBE Range: -1.0 - 1500.0  
 Apply N Rule: no  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

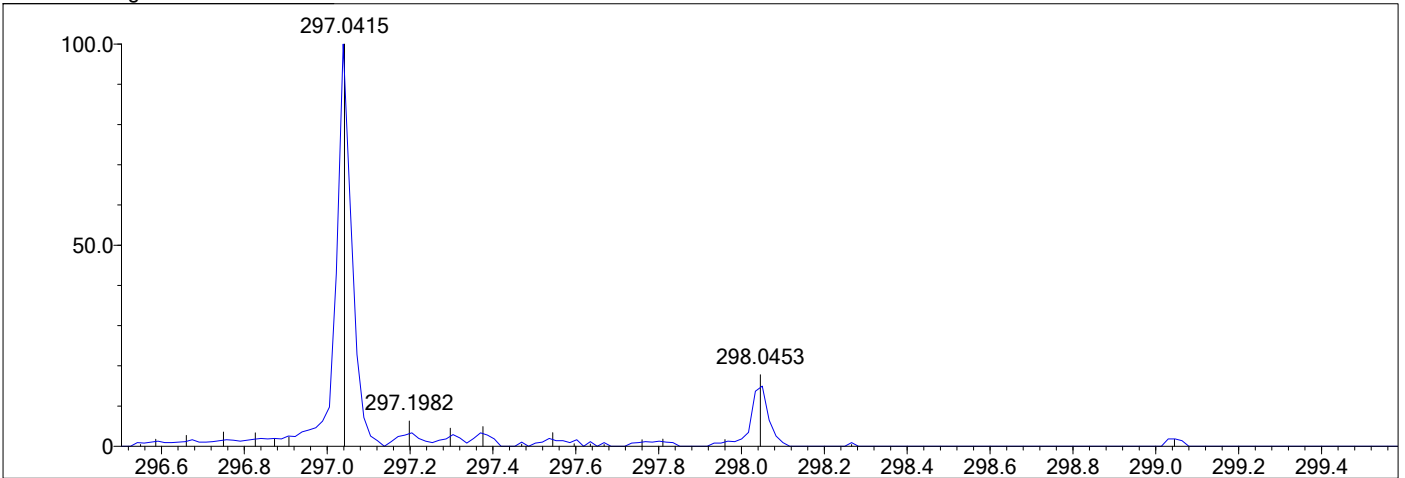
Electron Ions: both  
 Use MSn Info: no  
 Isotope Res: 10000  
 Max Results: 40

Event#: 2 MS(E-) Ret. Time : 0.653 Scan#: 100

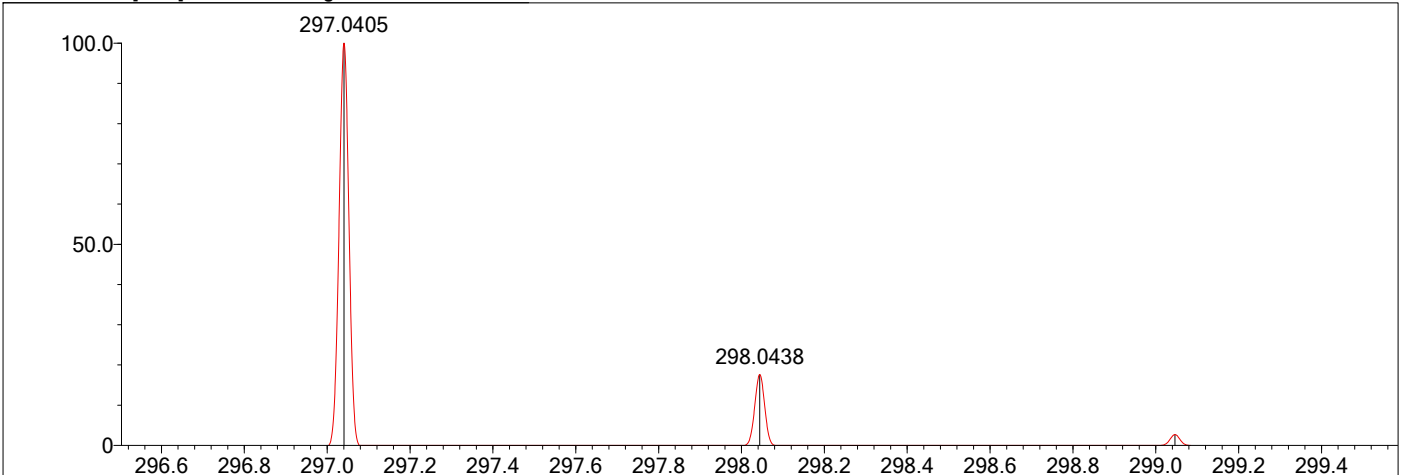
2v



Measured region for 297.0415 m/z



C16 H10 O6 [M-H]-: Predicted region for 297.0405 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	79.26	C16 H10 O6	[M-H]-	297.0415	297.0405	1.0	3.37	84.25	12.0

Data File: F:\高分辨数据\Zouyong\SXH\SJF-4S.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	8	N	3	0	0	P	3	0	0	Br	1	0	0	H
B	3	0	0	O	2	0	4	S	2	0	0	I	3	0	0	HCOO
C	4	0	8	F	1	0	0	Cl	1	0	0					CH3COO

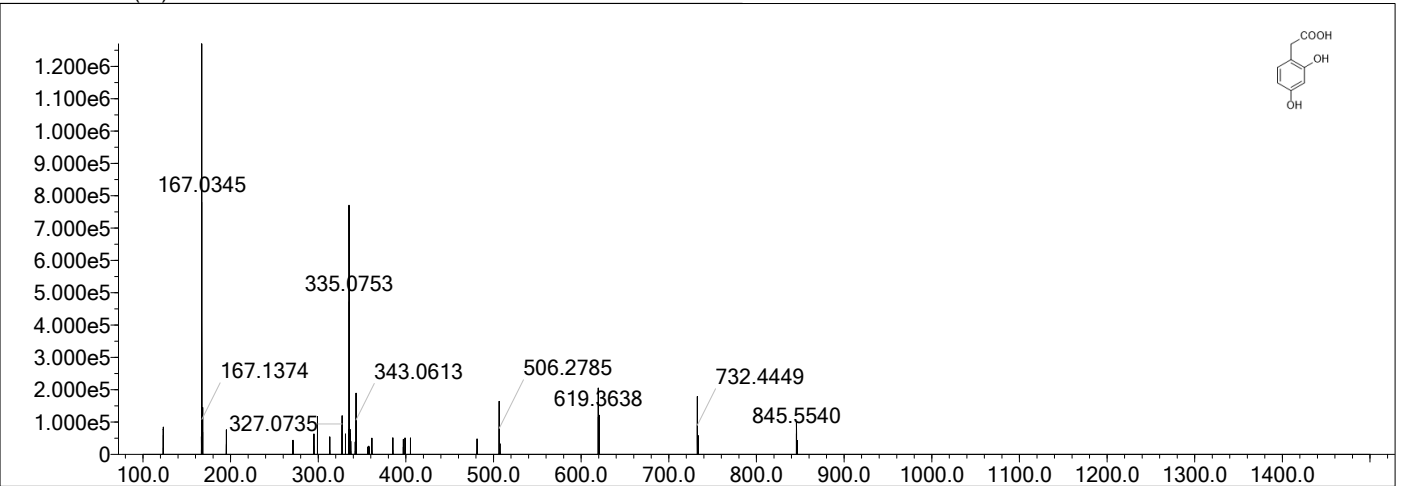
Error Margin (ppm): 20  
 HC Ratio: unlimited  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

DBE Range: -1.0 - 1500.0  
 Apply N Rule: no  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

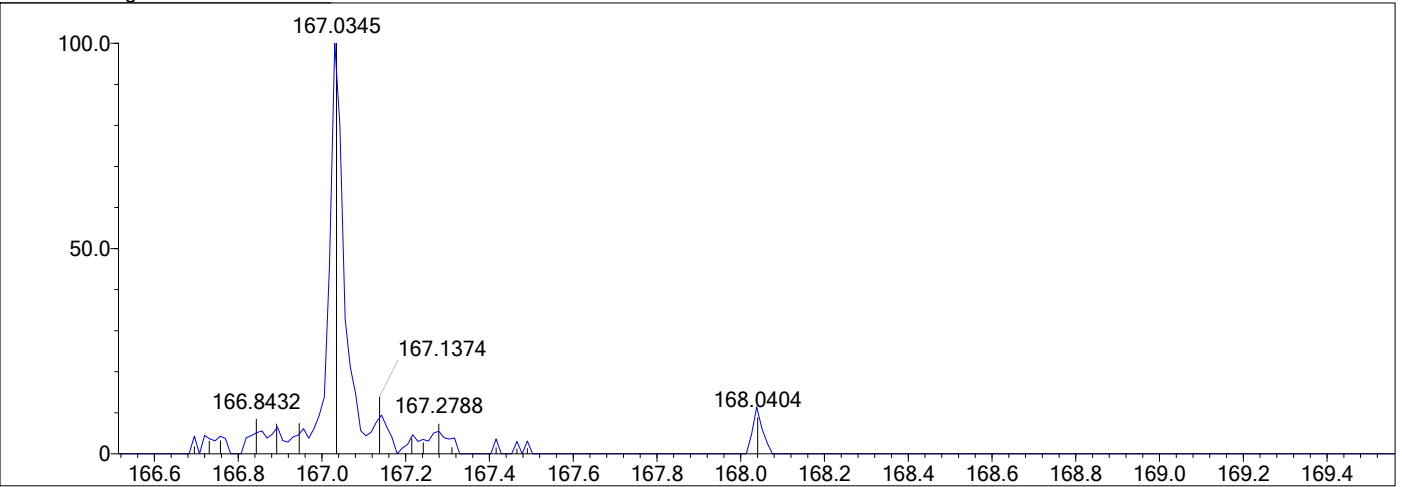
Electron Ions: both  
 Use MSn Info: no  
 Isotope Res: 10000  
 Max Results: 40

Event#: 2 MS(E-) Ret. Time : 0.680 - 0.587 -> 0.975 Scan#: 104 - 90 -> 148

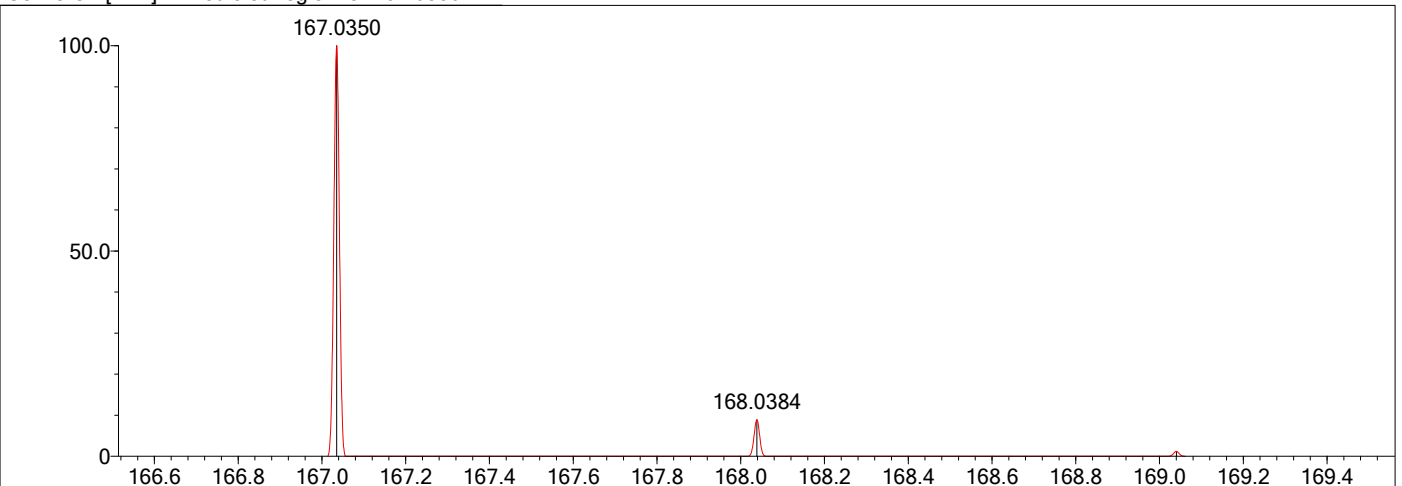
4s



Measured region for 167.0345 m/z



C8 H8 O4 [M-H]- : Predicted region for 167.0350 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	45.78	C8 H8 O4	[M-H]-	167.0345	167.0350	-0.5	-2.99	48.18	5.0

Data File: F:\高分辨数据\Zouyong\SXH\SJF-4T.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	7	10	N	3	0	0	P	3	0	0	Br	1	0	0	H
B	3	0	0	O	2	0	4	S	2	0	0	I	3	0	0	HCOO
C	4	8	9	F	1	0	0	Cl	1	0	0					

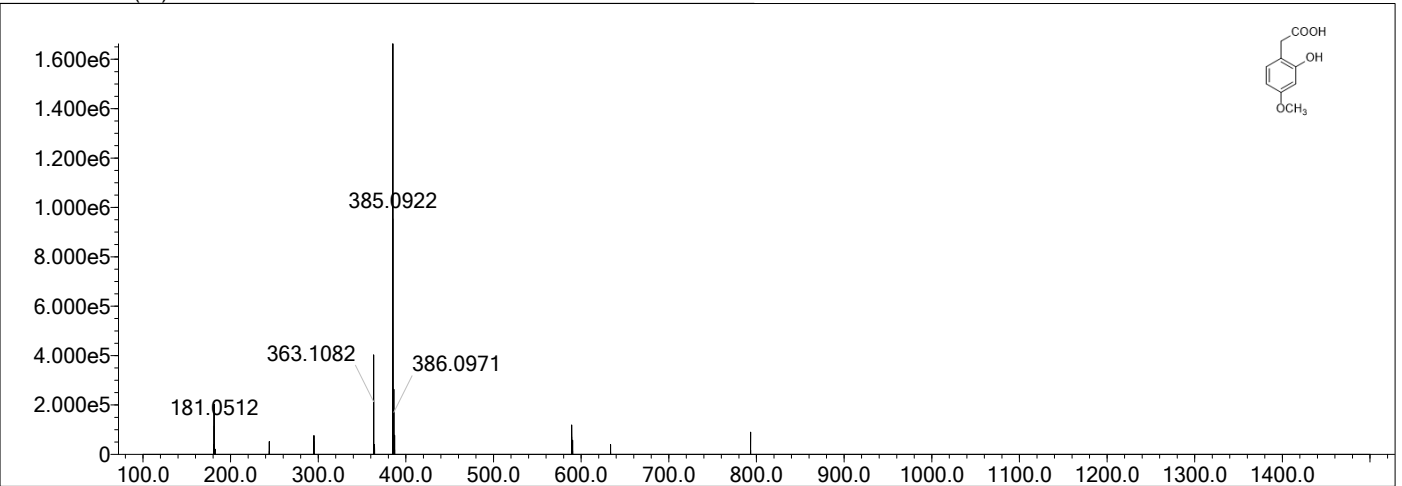
Error Margin (ppm): 100  
 HC Ratio: unlimited  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

DBE Range: -1.0 - 1500.0  
 Apply N Rule: no  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

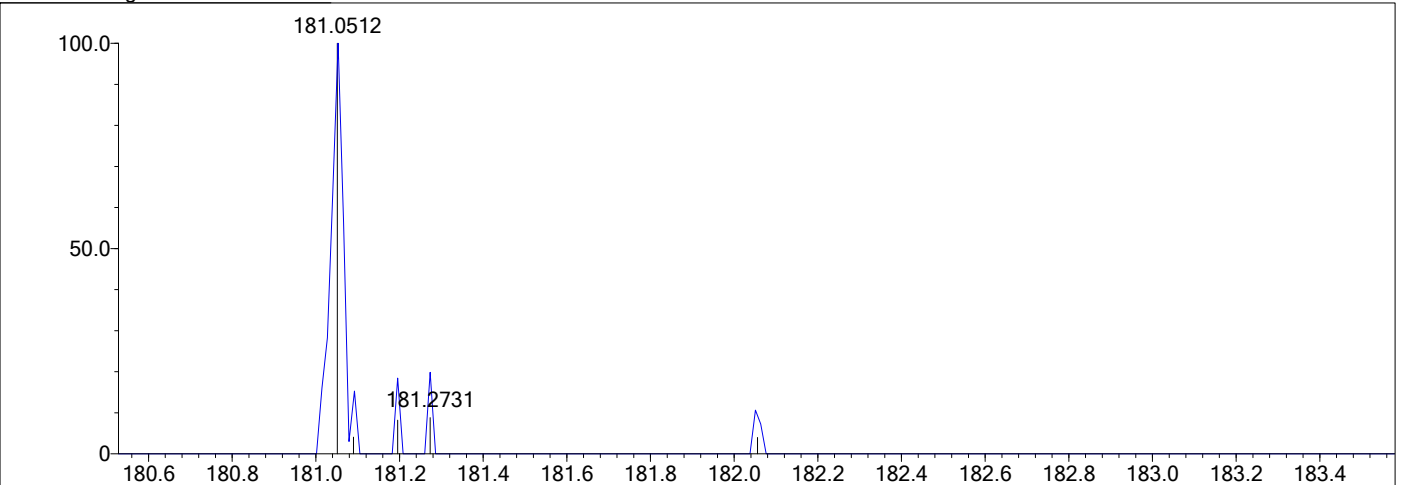
Electron Ions: both  
 Use MSn Info: no  
 Isotope Res: 10000  
 Max Results: 40

Event#: 2 MS(E-) Ret. Time : 1.013 - 0.733 -> 2.219 Scan#: 154 - 112 -> 334

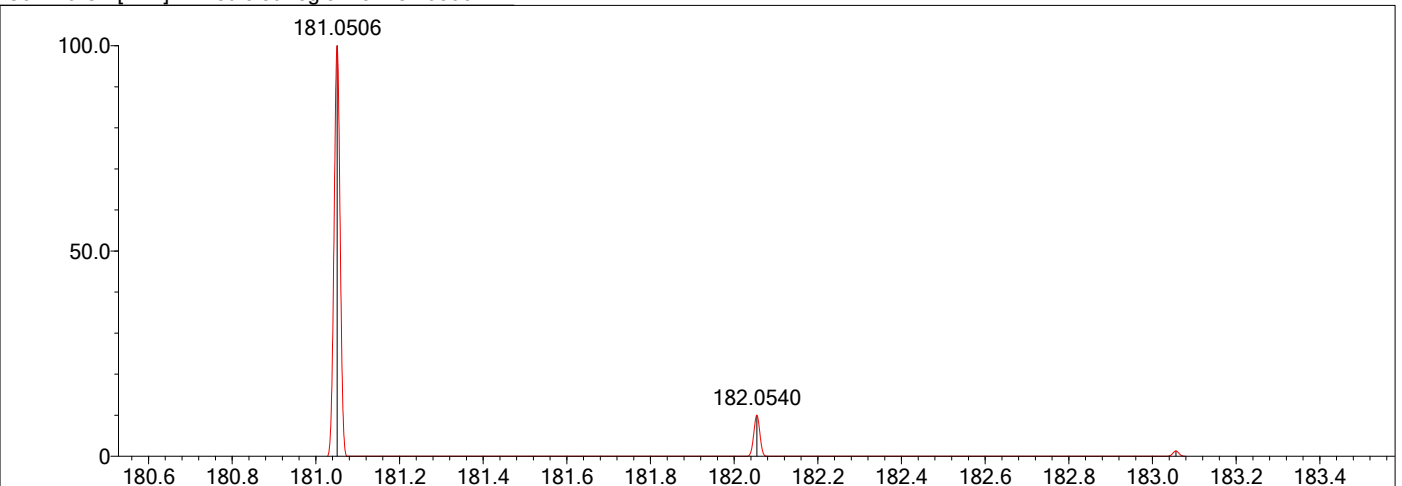
4t



Measured region for 181.0512 m/z



C9 H10 O4 [M-H]- : Predicted region for 181.0506 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	58.19	C9 H10 O4	[M-H]-	181.0512	181.0506	0.6	3.31	61.75	5.0



Data File: F:\高分辨数据\Zouyong\SXH\SJF-4U.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	11	12	N	3	0	0	P	3	0	0	Br	1	0	0	H
B	3	0	0	O	2	0	5	S	2	0	0	I	3	0	0	HCOO
C	4	10	10	F	1	0	0	Cl	1	0	0					

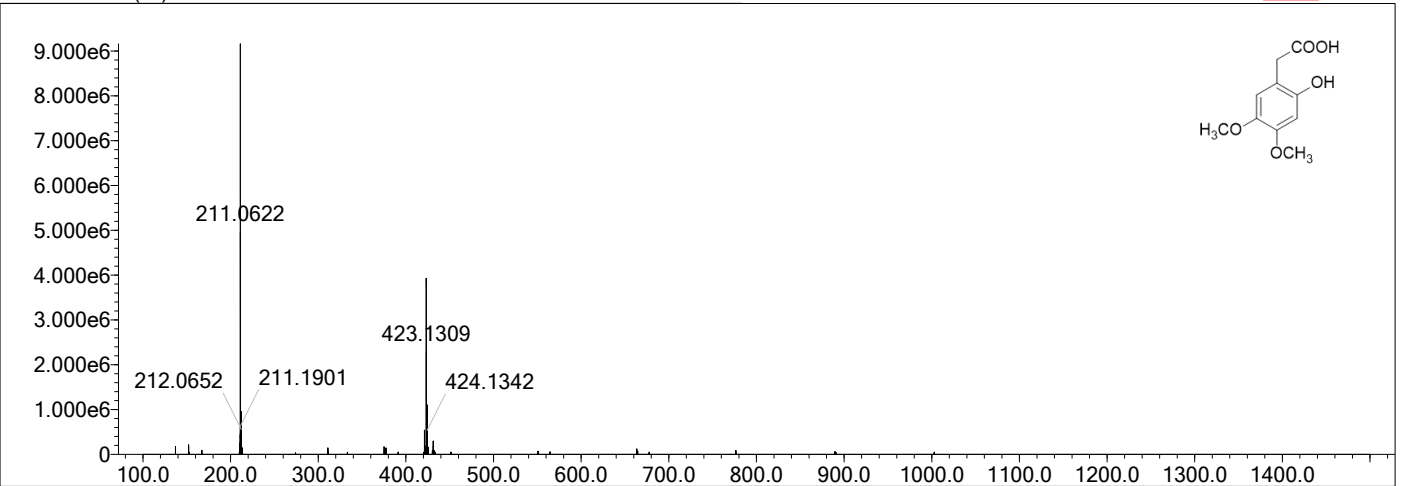
Error Margin (ppm): 100  
 HC Ratio: unlimited  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

DBE Range: -1.0 - 1500.0  
 Apply N Rule: no  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

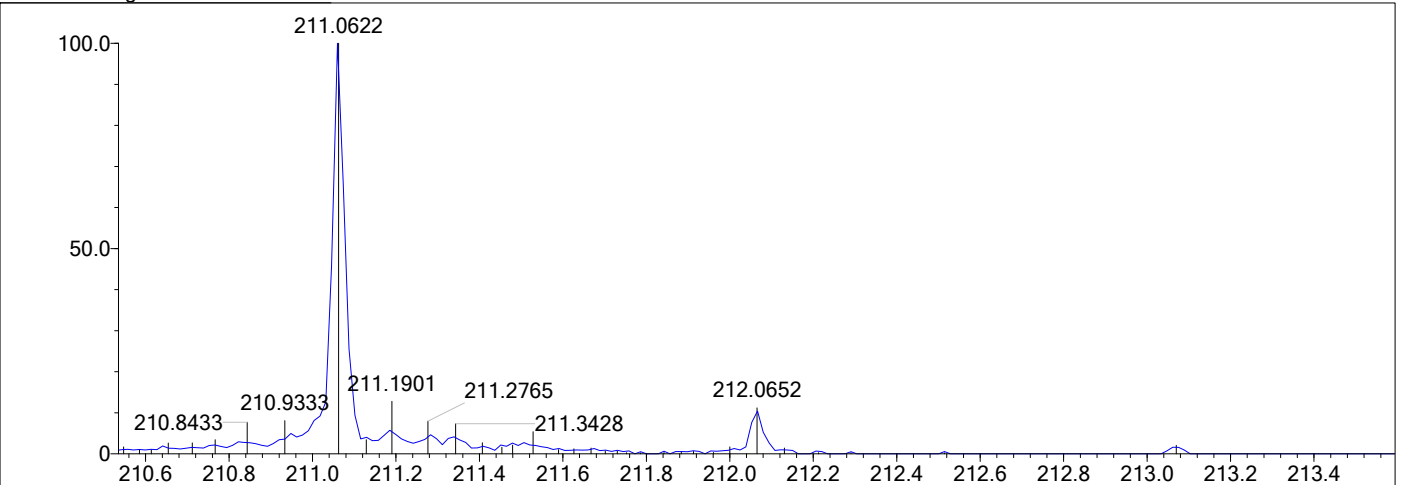
Electron Ions: both  
 Use MSn Info: no  
 Isotope Res: 10000  
 Max Results: 40

4u

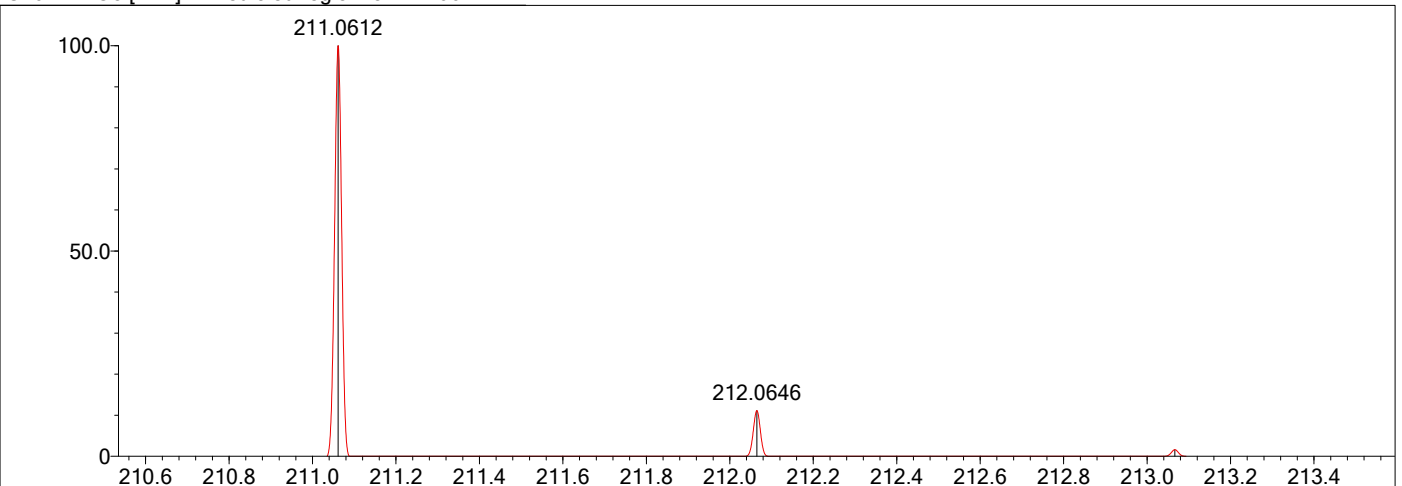
Event#: 2 MS(E-) Ret. Time : 0.680 - 0.573 -> 1.855 Scan#: 104 - 88 -> 280



Measured region for 211.0622 m/z



C10 H12 O5 [M-H]- : Predicted region for 211.0612 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	78.59	C10 H12 O5	[M-H]-	211.0622	211.0612	1.0	4.74	86.70	5.0

Data File: F:\高分辨数据\Zouyong\SXH\SJF-4V.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	8	N	3	0	0	P	3	0	0	Br	1	0	0	H
B	3	0	0	O	2	0	5	S	2	0	0	I	3	0	0	HCOO
C	4	0	9	F	1	0	0	Cl	1	0	0					

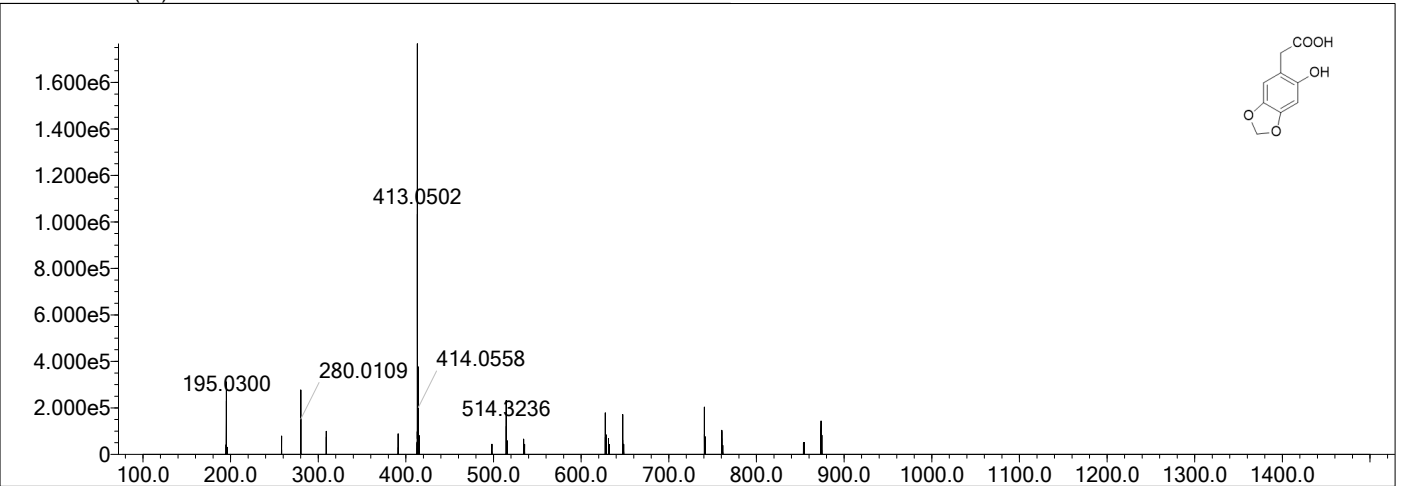
Error Margin (ppm): 50  
 HC Ratio: unlimited  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

DBE Range: -1.0 - 1500.0  
 Apply N Rule: no  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

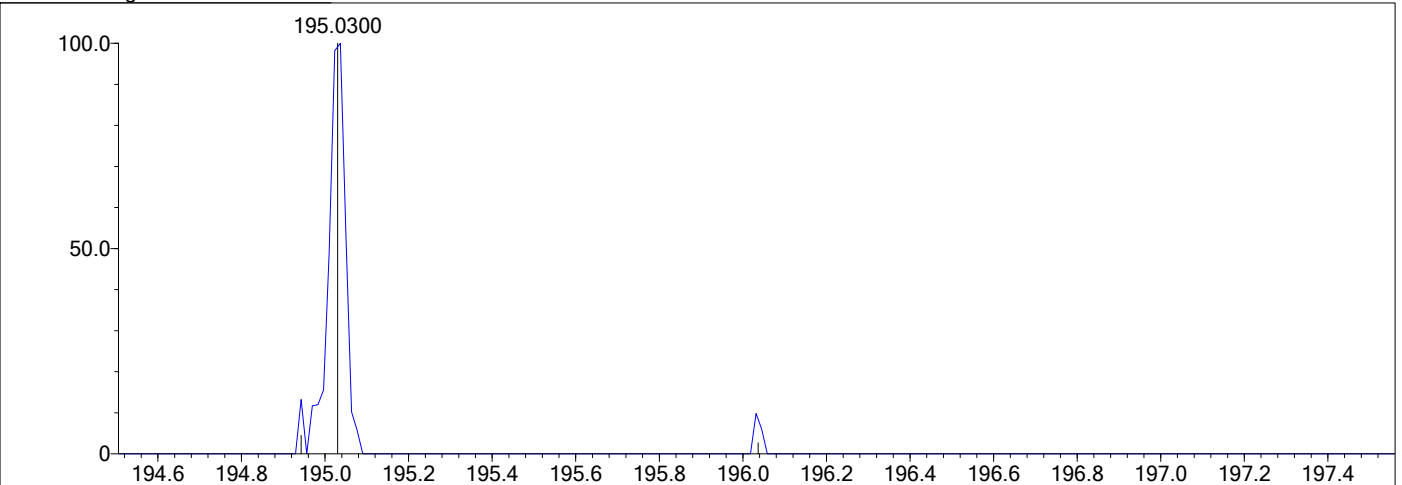
Electron Ions: both  
 Use MSn Info: no  
 Isotope Res: 10000  
 Max Results: 40

4v

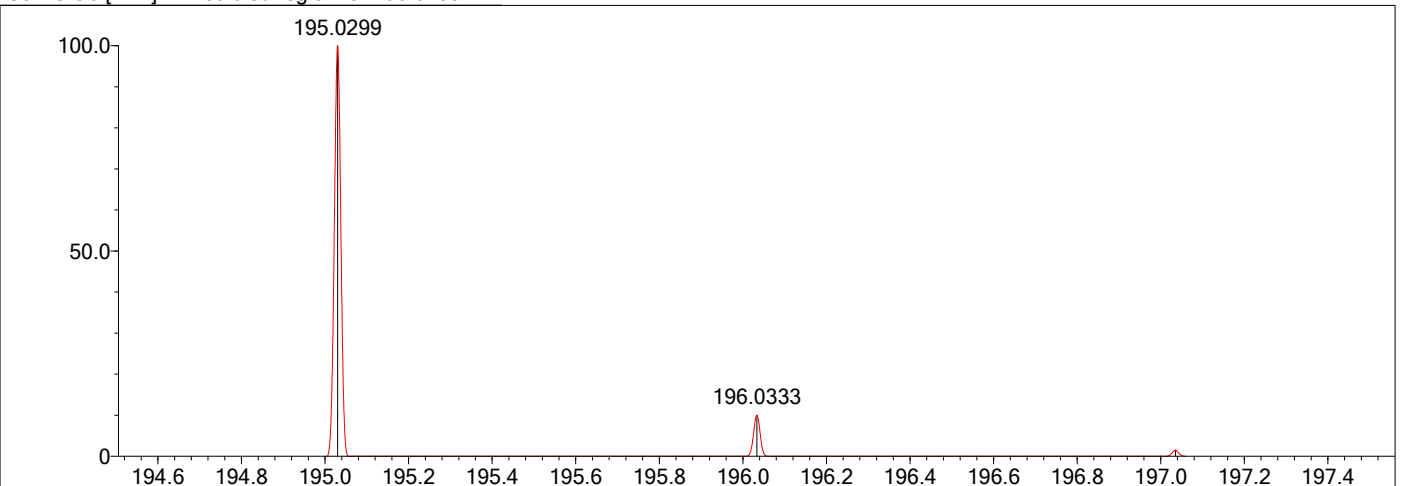
Event#: 2 MS(E-) Ret. Time : 0.600 - 0.333 -> 2.508 Scan# : 92 - 52 -> 378



Measured region for 195.0300 m/z



C9 H8 O5 [M-H]- : Predicted region for 195.0299 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	82.26	C9 H8 O5	[M-H]-	195.0300	195.0299	0.1	0.51	82.26	6.0

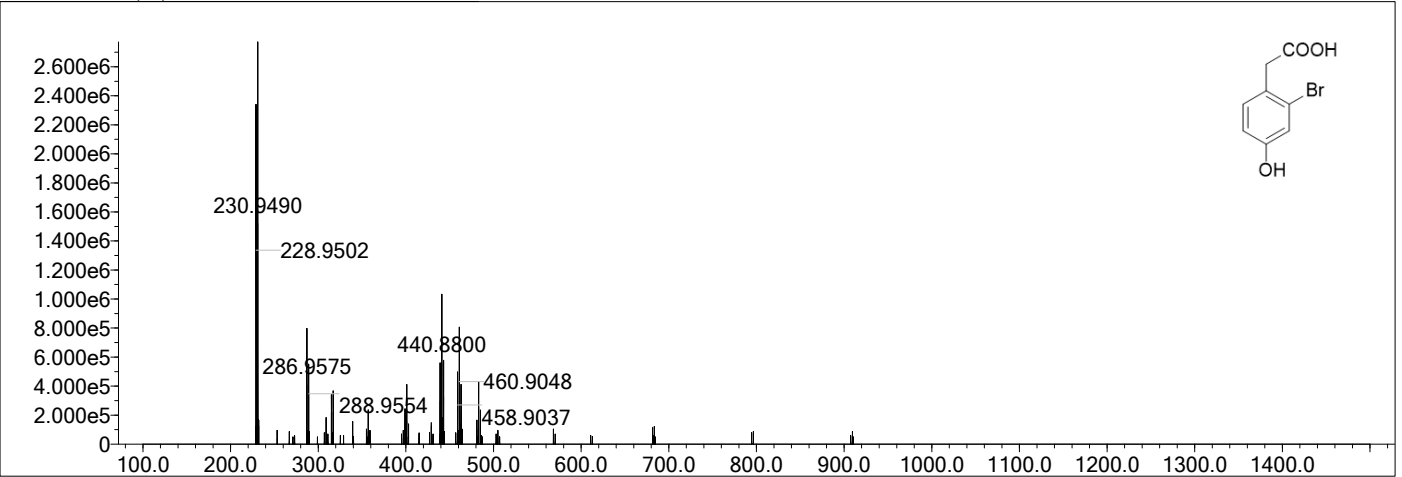
Data File: F:\高分辨数据\Zouyong\SXH\SJF-5S.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	11	O	2	0	3	Cl	1	0	0	H
B	3	0	0	F	1	0	0	Br	1	0	1	HCOO
C	4	0	10	P	3	0	0	I	3	0	0	CH3COO
N	3	0	0	S	2	0	0					Cl

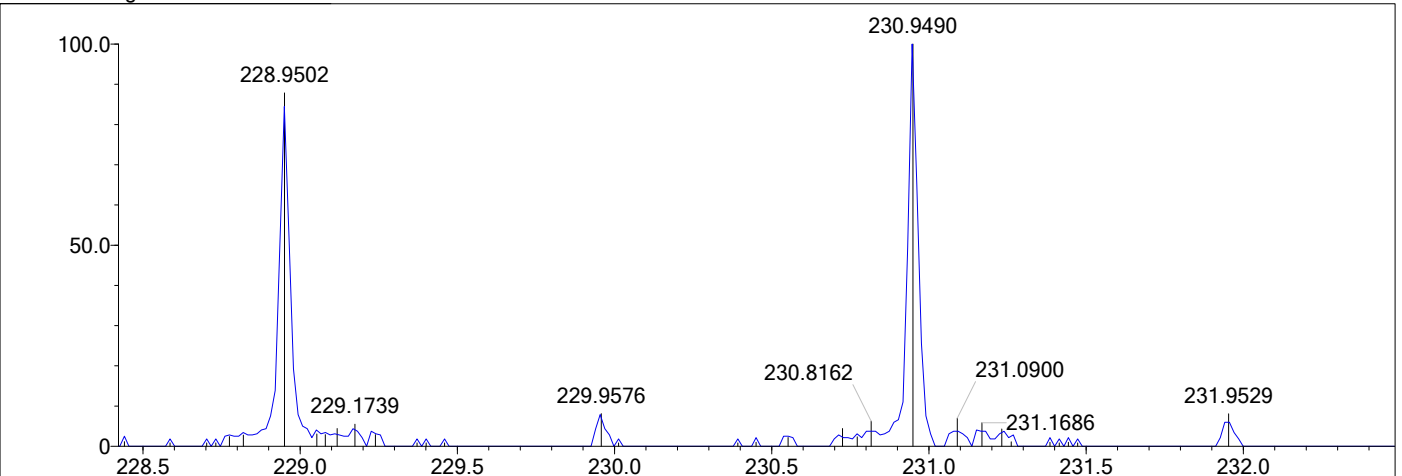
Error Margin (ppm): 5  
 DBE Range: -1.0 - 1500.0  
 Electron Ions: both  
 HC Ratio: unlimited  
 Apply N Rule: no  
 Use MSn Info: no  
 Max Isotopes: all  
 Isotope RI (%): 1.00  
 Isotope Res: 10000  
 MSn Iso RI (%): 75.00  
 MSn Logic Mode: AND  
 Max Results: 40

5s

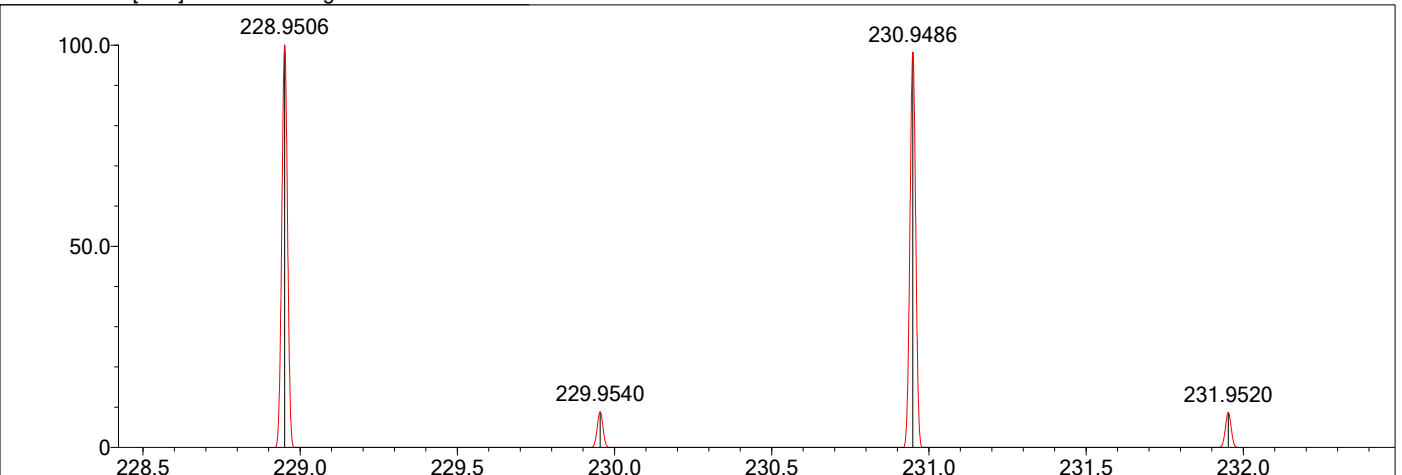
Event#: 2 MS(E-) Ret. Time : 0.733 Scan#: 112



Measured region for 228.9502 m/z



C8 H7 O3 Br [M-H]- : Predicted region for 228.9506 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	47.75	C8 H7 O3 Br	[M-H]-	228.9502	228.9506	-0.4	-1.75	48.66	5.0

Data File: F:\高分辨数据\Zouyong\SXH\SJF-5U.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	11	11	N	3	0	0	P	3	0	0	Br	1	0	1	H
B	3	0	0	O	2	0	4	S	2	0	0	I	3	0	0	HCOO
C	4	10	10	F	1	0	0	Cl	1	0	0					

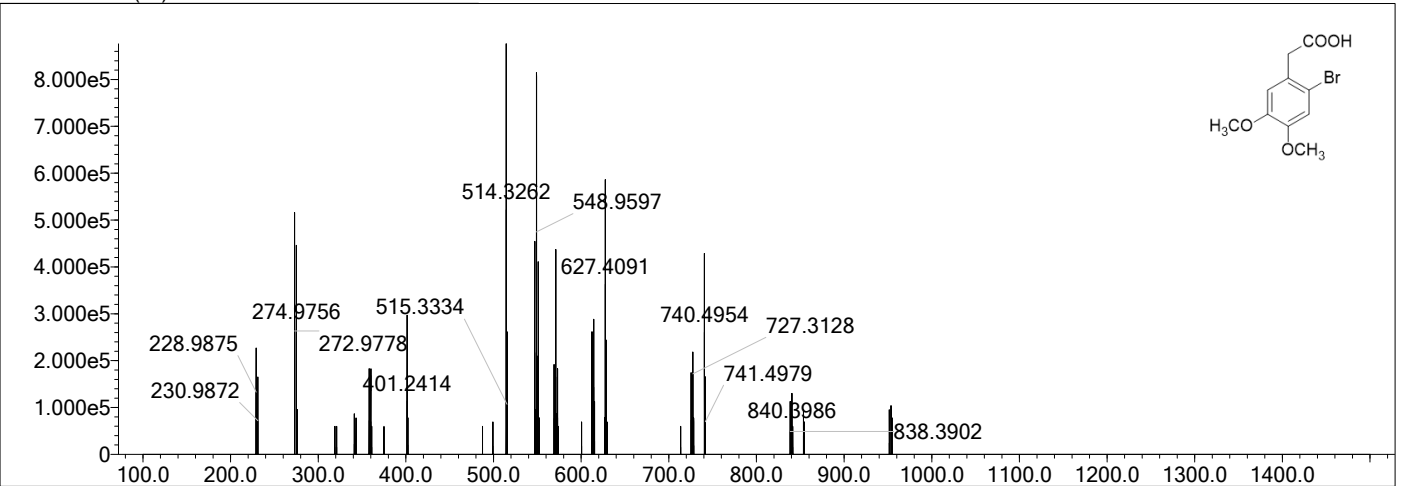
Error Margin (ppm): 100  
 HC Ratio: unlimited  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

DBE Range: -1.0 - 1500.0  
 Apply N Rule: no  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

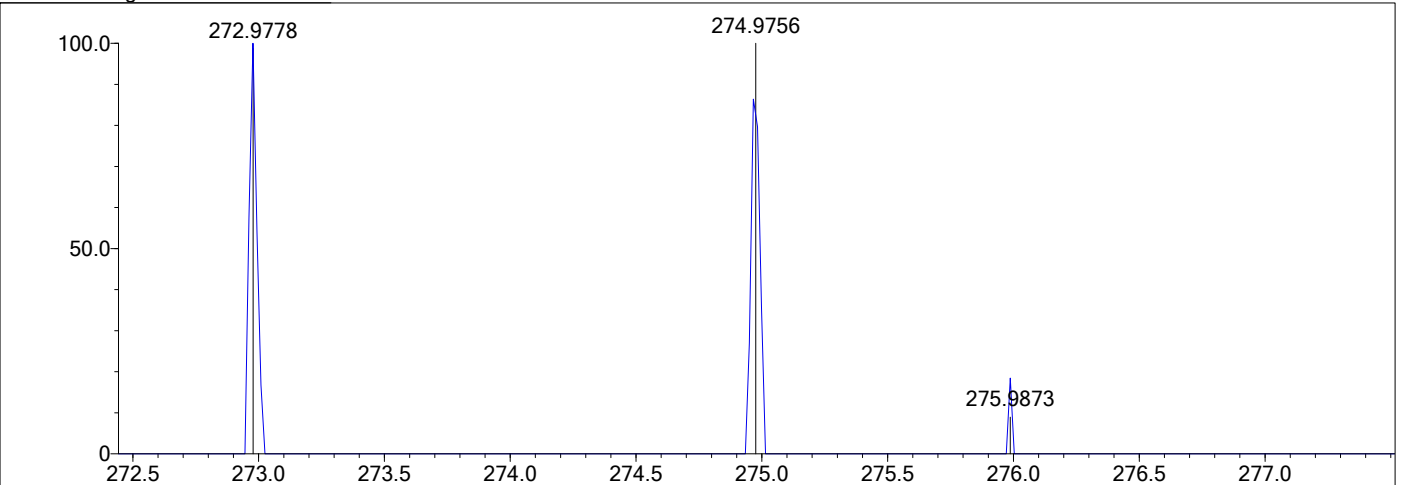
Electron Ions: both  
 Use MSn Info: no  
 Isotope Res: 10000  
 Max Results: 40

Event#: 2 MS(E-) Ret. Time : 0.720 Scan#: 110

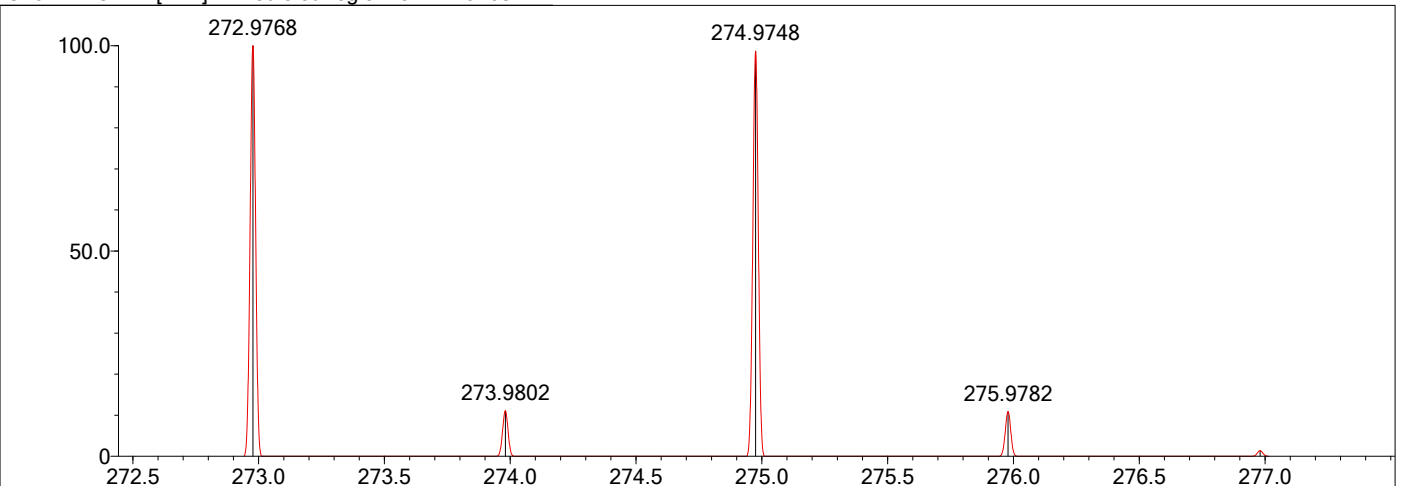
5u



Measured region for 272.9778 m/z



C10 H11 O4 Br [M-H]- : Predicted region for 272.9768 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	28.15	C10 H11 O4 Br	[M-H]-	272.9778	272.9768	1.0	3.66	30.16	5.0

Data File: F:\高分辨数据\Zouyong\SXH\SJF-5V.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	7	O	2	0	4	Cl	1	0	0	H
B	3	0	0	F	1	0	0	Br	1	0	1	HCOO
C	4	0	9	P	3	0	0	I	3	0	0	CH3COO
N	3	0	0	S	2	0	0					Cl

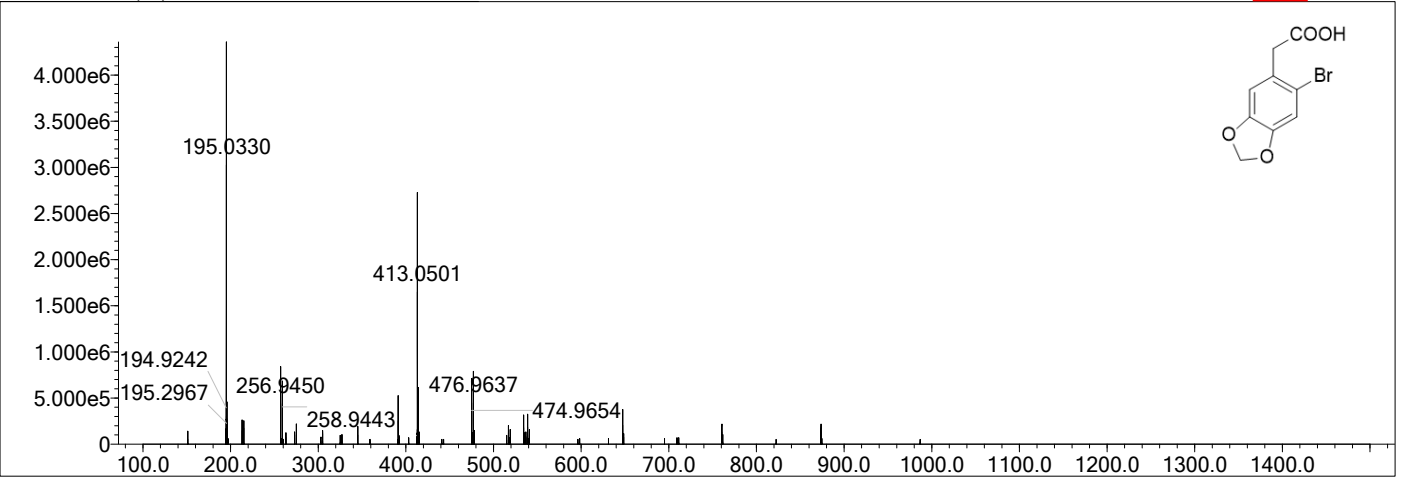
Error Margin (ppm): 5  
 HC Ratio: unlimited  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

DBE Range: -1.0 - 1500.0  
 Apply N Rule: no  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

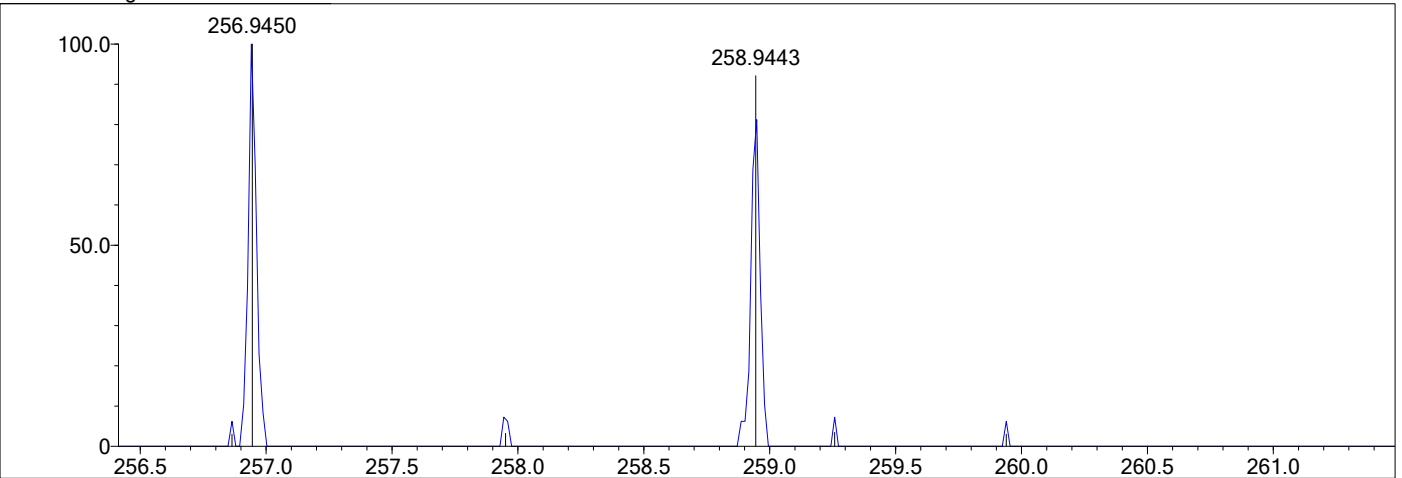
Electron Ions: both  
 Use MSn Info: no  
 Isotope Res: 10000  
 Max Results: 40

Event#: 2 MS(E-) Ret. Time : 0.707 Scan# : 108

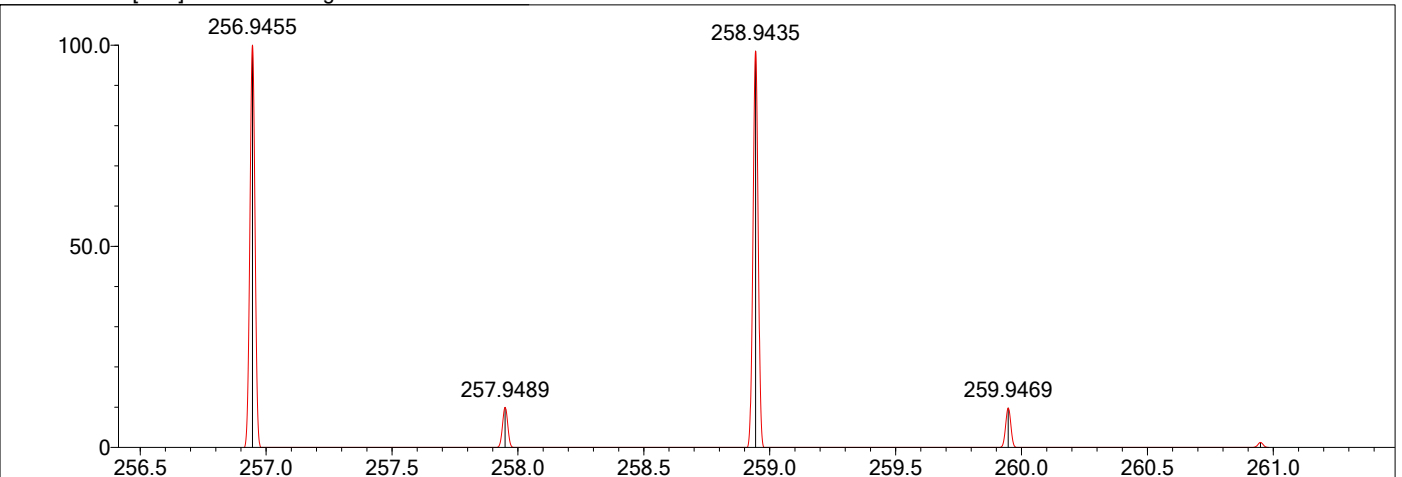
5v



Measured region for 256.9450 m/z



C9 H7 O4 Br [M-H]- : Predicted region for 256.9455 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	28.41	C9 H7 O4 Br	[M-H]-	256.9450	256.9455	-0.5	-1.95	29.10	6.0

Data File: F:\高分辨数据\Zouyong\SXH\SJF-7.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	7	7	N	3	0	0	P	3	0	0	Br	1	0	1	H
B	3	0	0	O	2	0	4	S	2	0	0	I	3	0	0	HCOO
C	4	8	8	F	1	0	0	Cl	1	0	0					

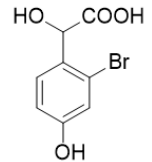
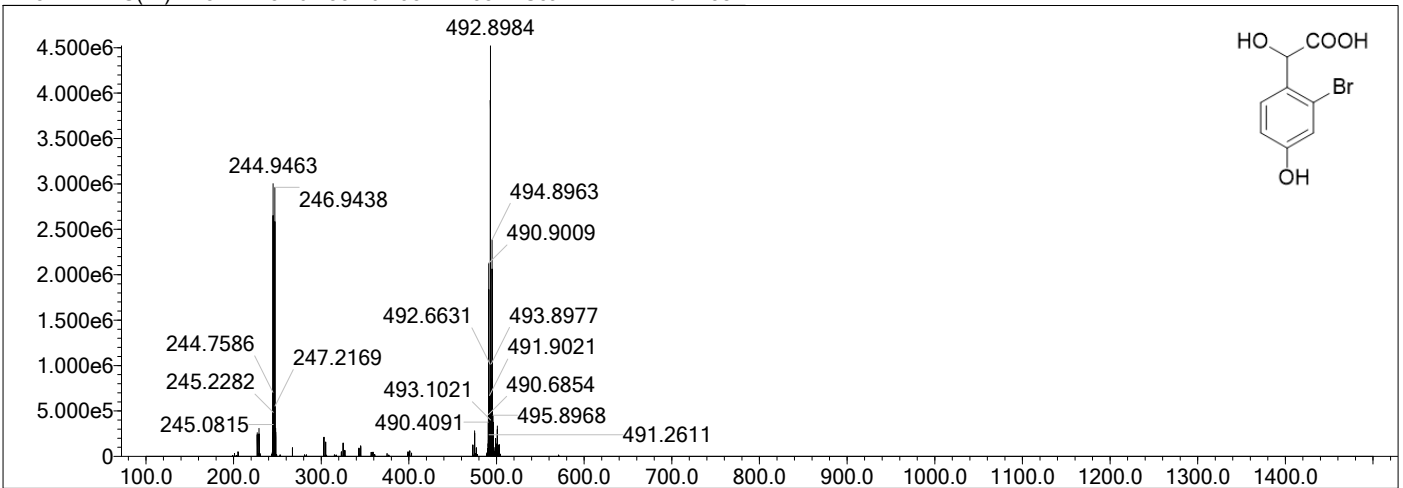
Error Margin (ppm): 100  
 HC Ratio: unlimited  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

DBE Range: -1.0 - 1500.0  
 Apply N Rule: no  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

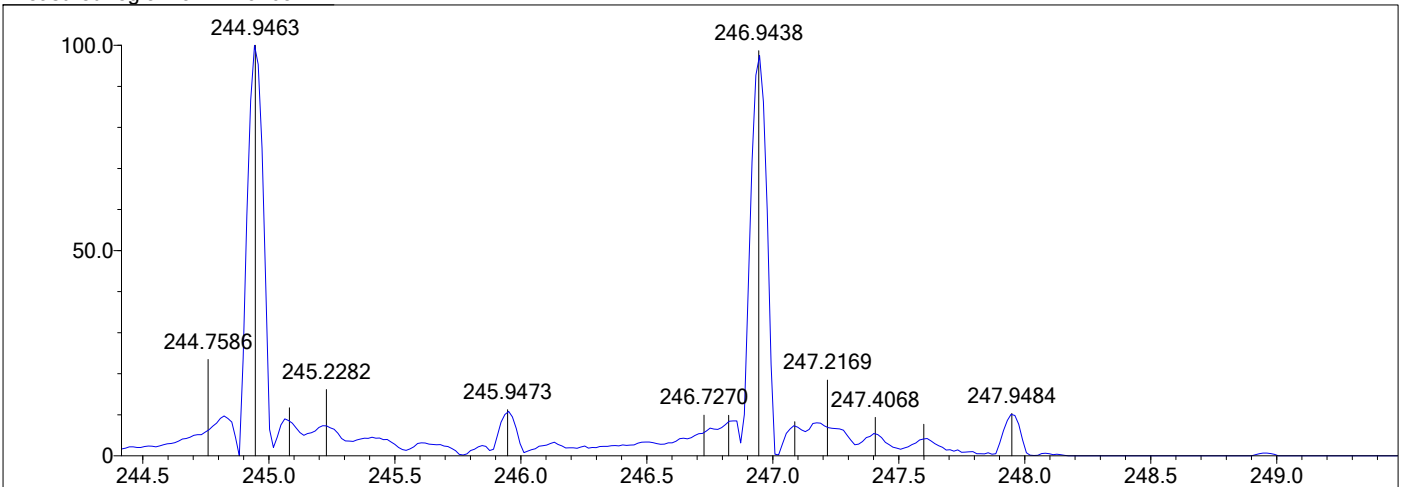
Electron Ions: both  
 Use MSn Info: no  
 Isotope Res: 10000  
 Max Results: 40

Event#: 2 MS(E-) Ret. Time : 0.733 - 0.493 -> 2.537 Scan#: 112 - 76 -> 382

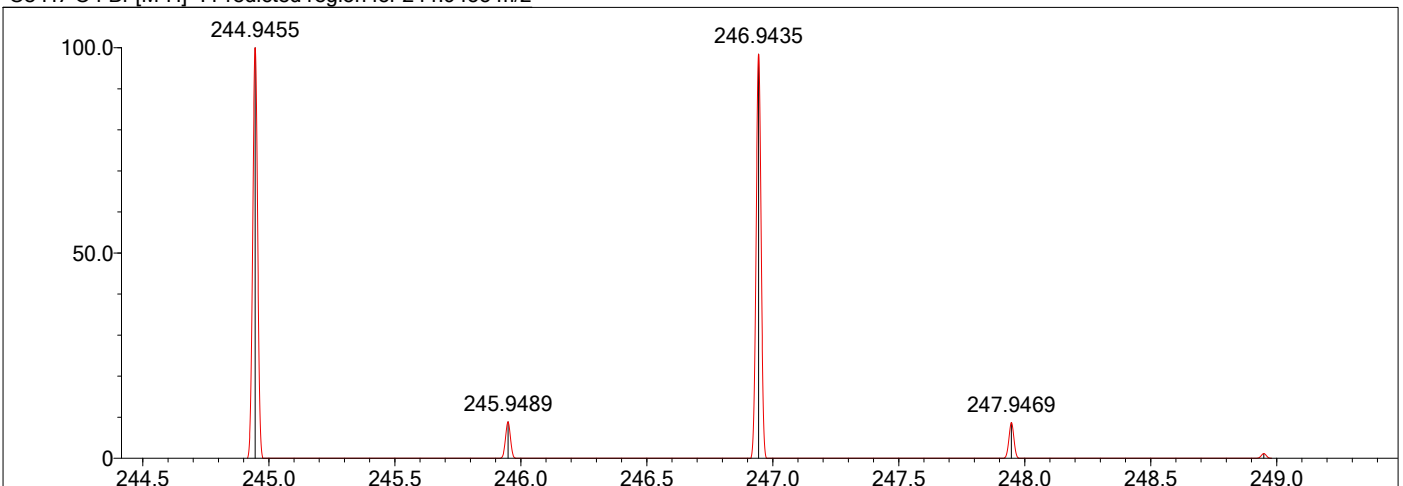
7



Measured region for 244.9463 m/z



C8 H7 O4 Br [M-H]- : Predicted region for 244.9455 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	80.24	C8 H7 O4 Br	[M-H]-	244.9463	244.9455	0.8	3.27	85.07	5.0

Data File: \\Deep-20160624\data1\邹永\SXH\SJF-2W.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	7	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	K
B	3	0	0	P	3	0	0	Cu	2	0	0	Au	1	0	0	
C	4	0	30	S	2	0	0	Se	2	0	0					
N	3	0	8	Cl	1	0	0	Br	1	0	0					

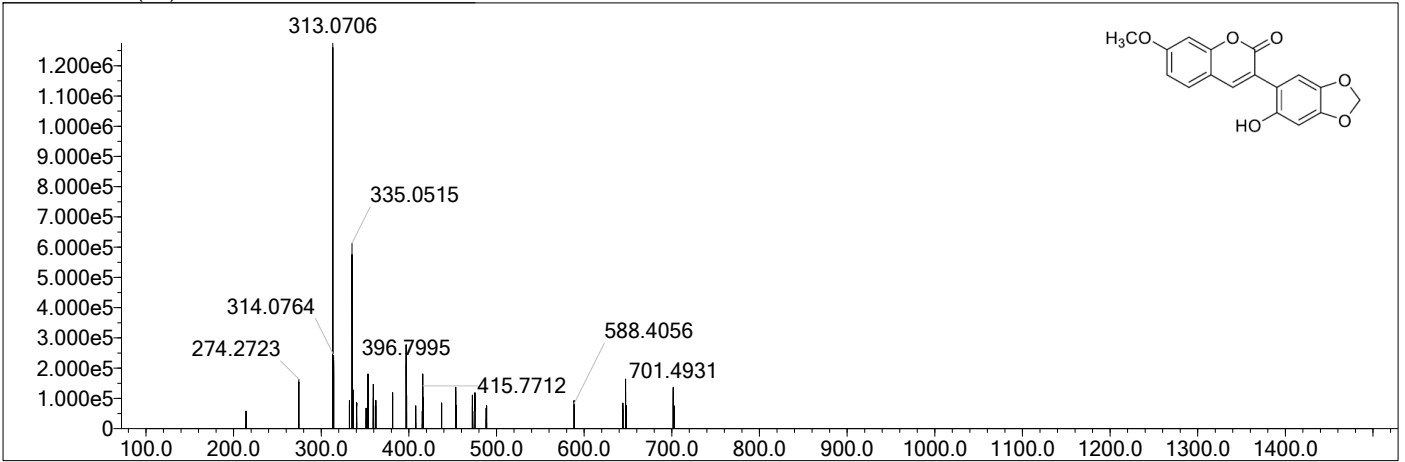
Error Margin (ppm): 50  
 HC Ratio: 0.0 - 20.0  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

DBE Range: -100.0 - 1000.0  
 Apply N Rule: yes  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

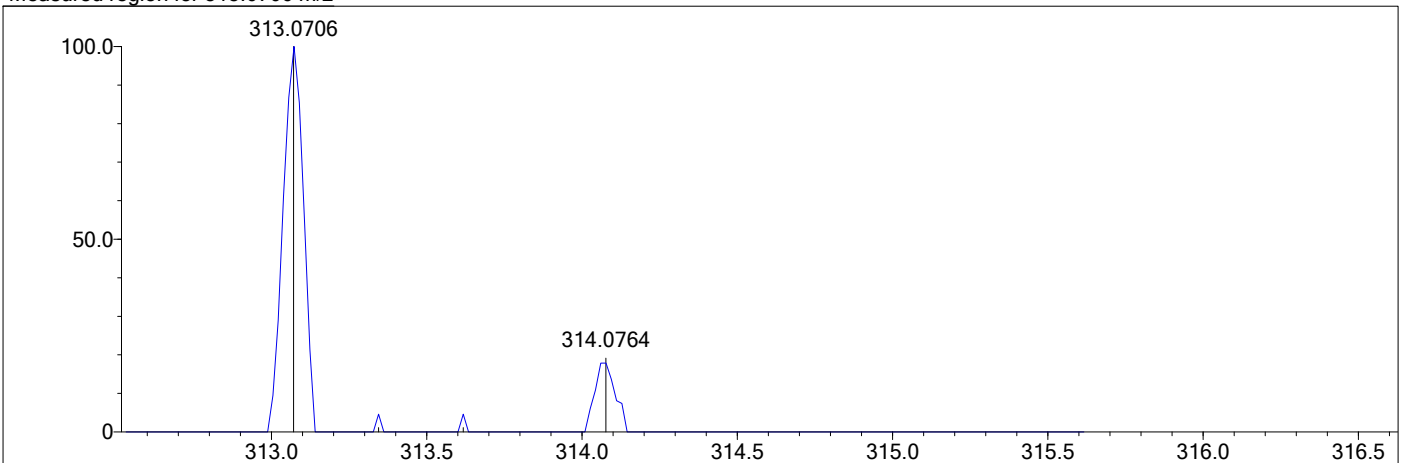
Electron Ions: both  
 Use MSn Info: no  
 Isotope Res: 10000  
 Max Results: 2000

Event#: 1 MS(E+) Ret. Time : 0.200 Scan#: 31

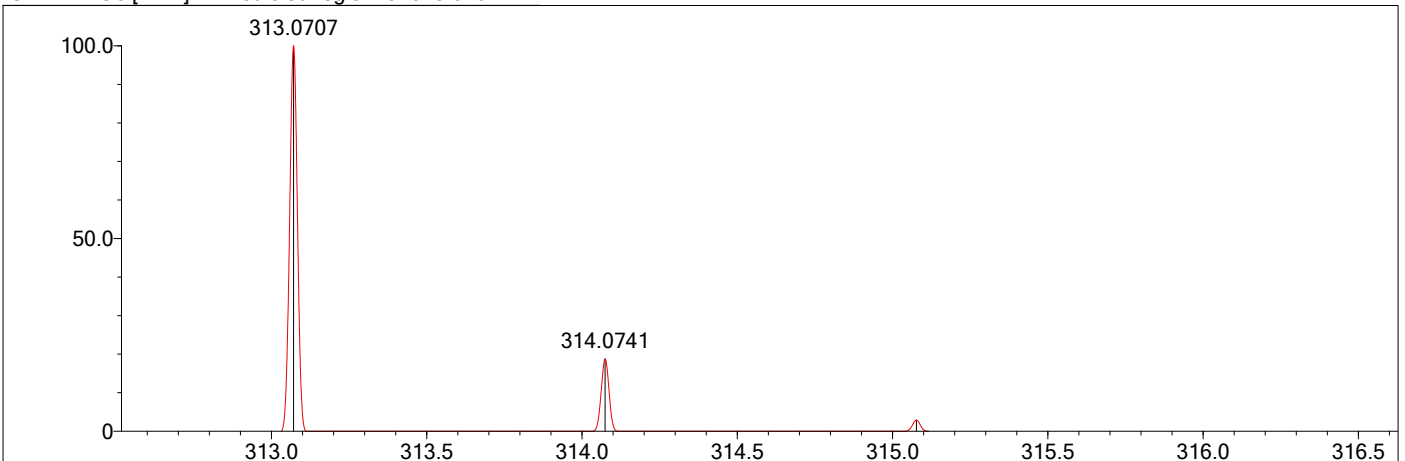
2w



Measured region for 313.0706 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	86.96	C17 H12 O6	[M+H] <sup>+</sup>	313.0706	313.0707	-0.1	-0.32	86.96	12.0