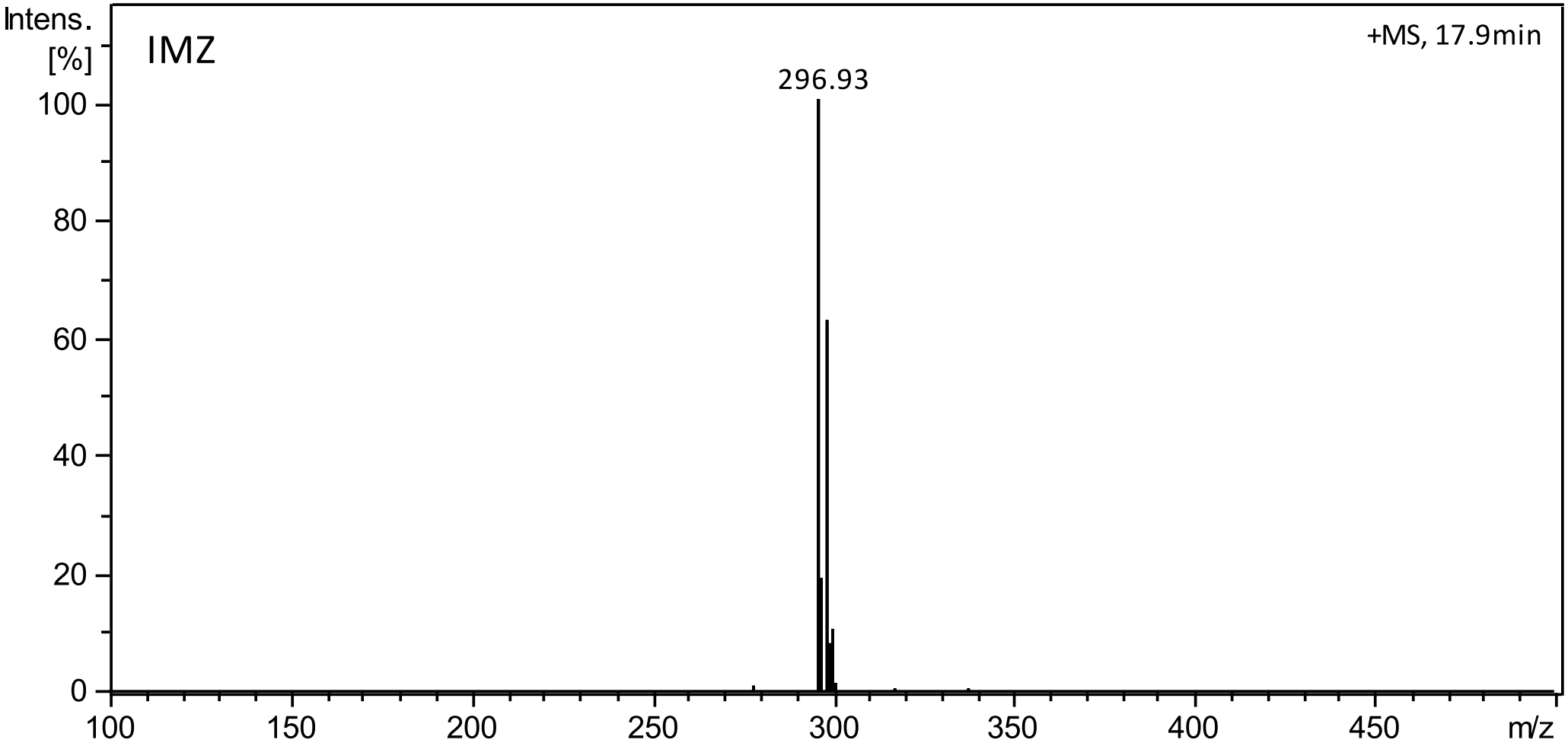
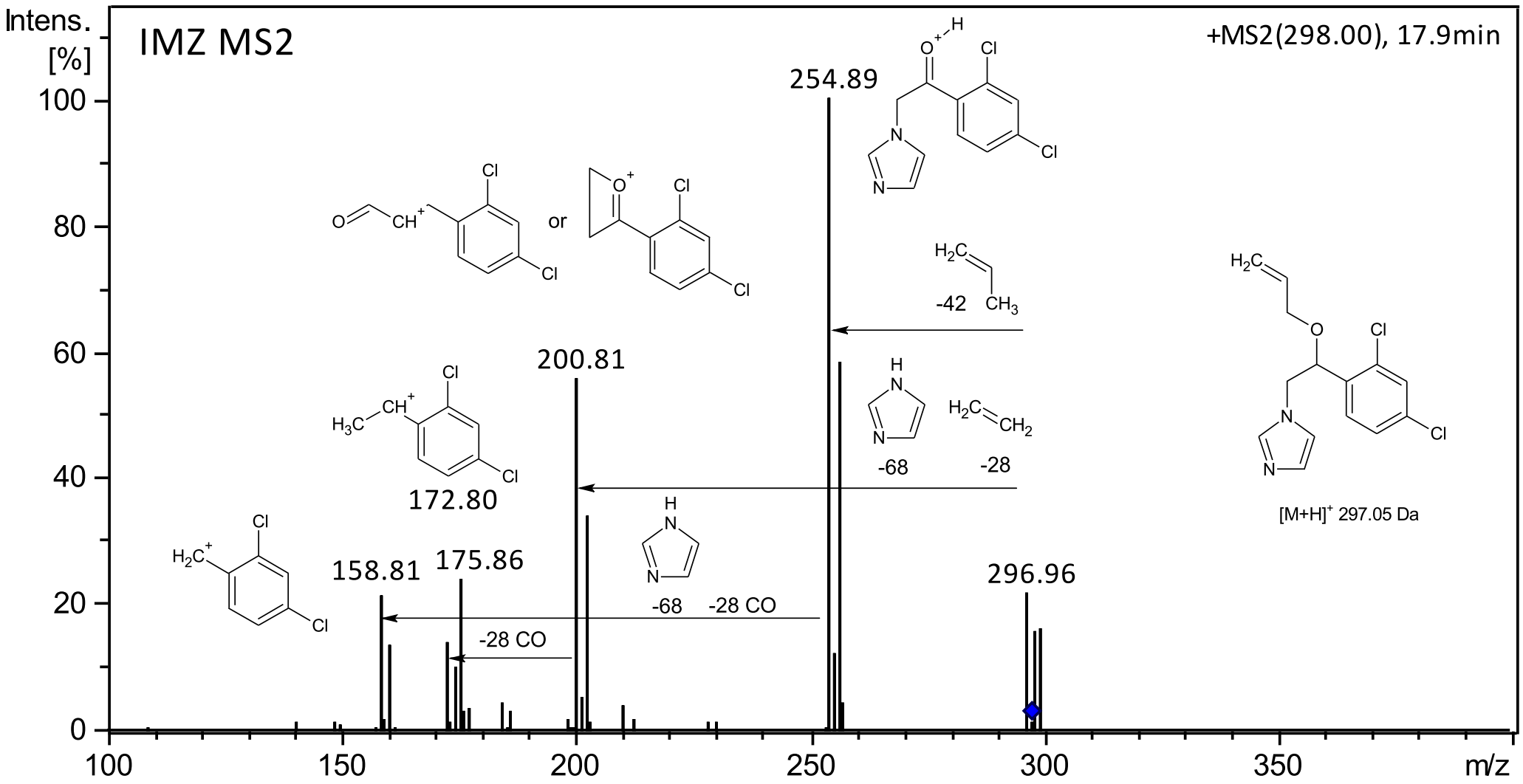
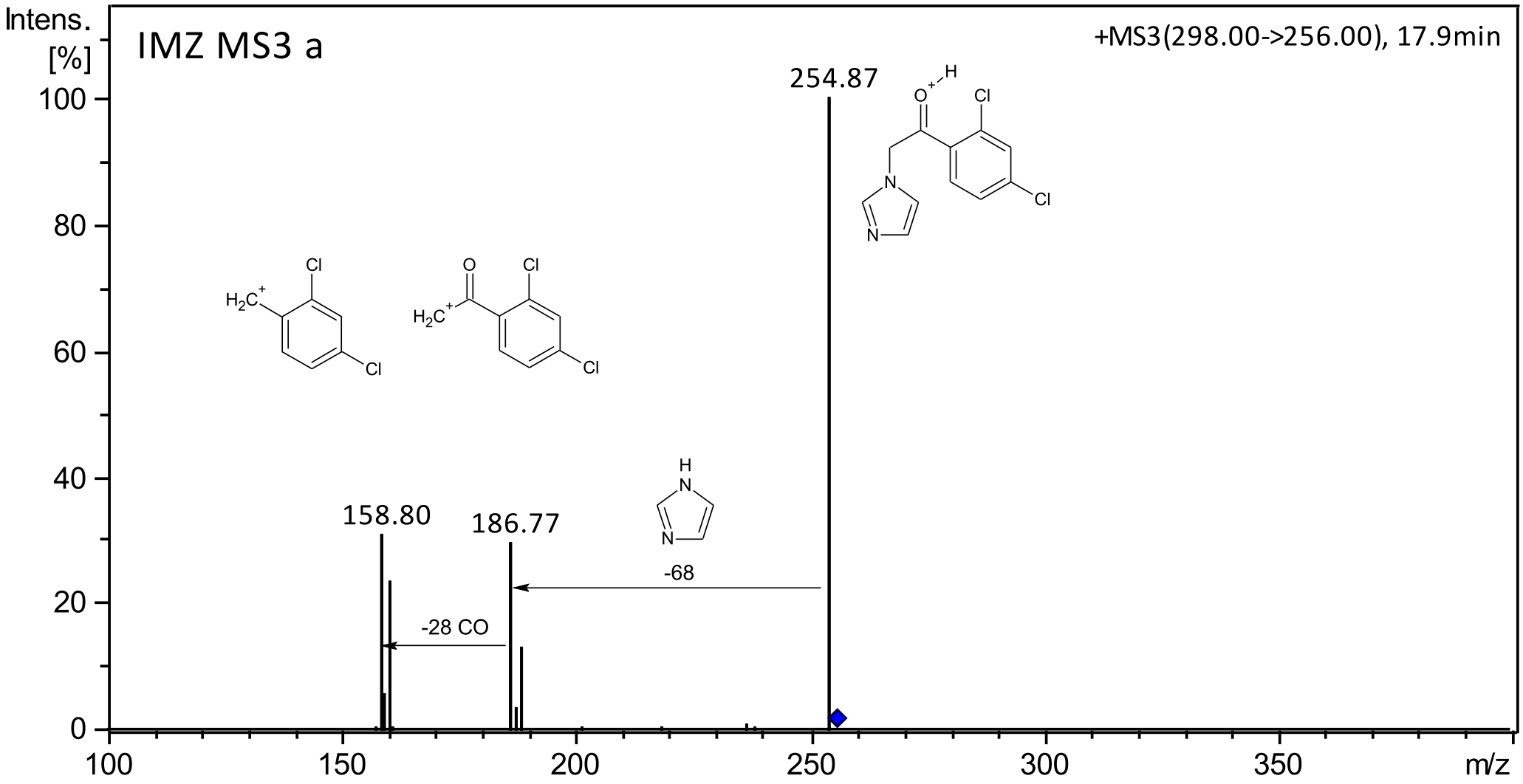
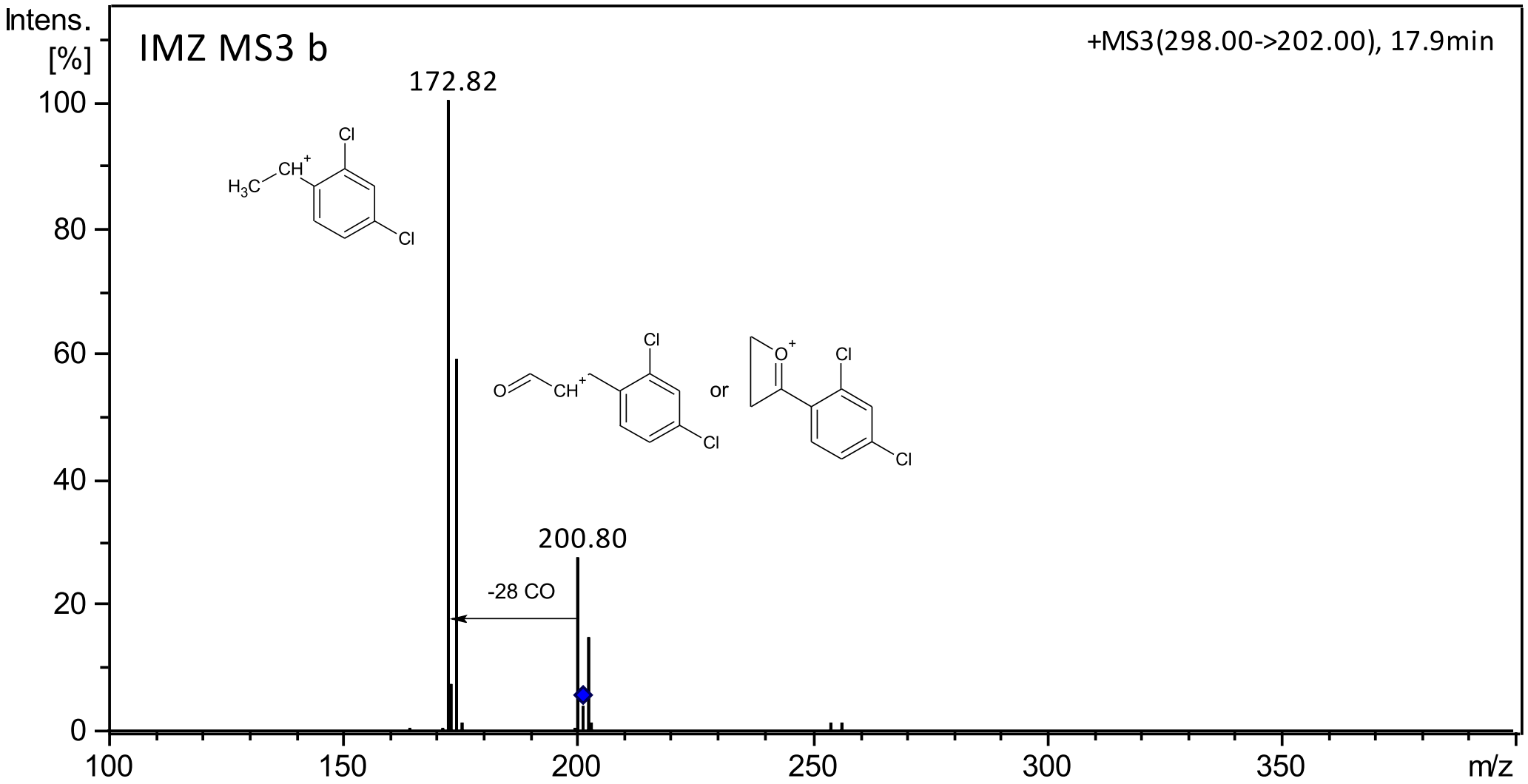
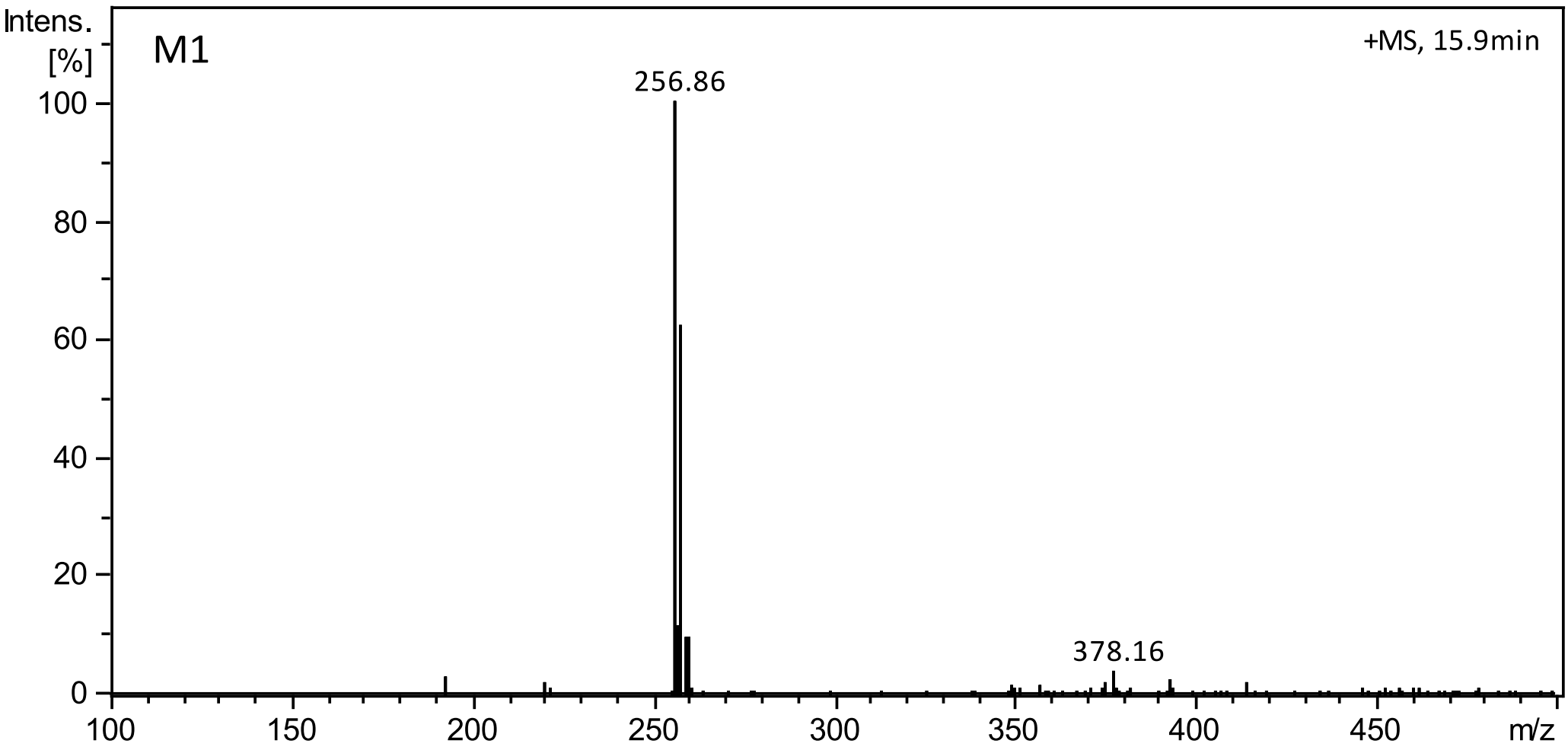
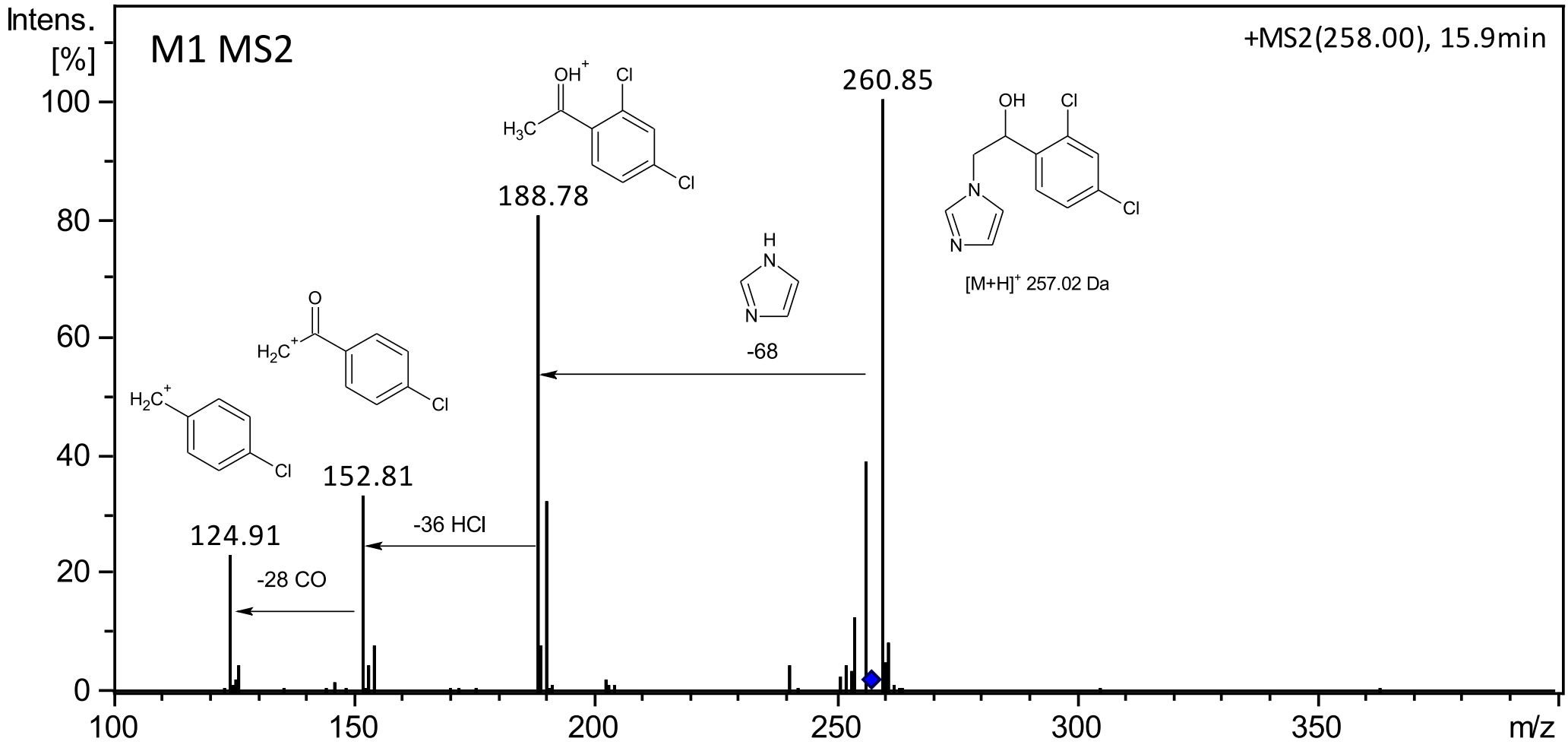

Intens.
[%]
IMZ
+MS, 17.9min
296.93
100
80
60
40
20
0
100
150
200
250
300
350
400
450
m/z

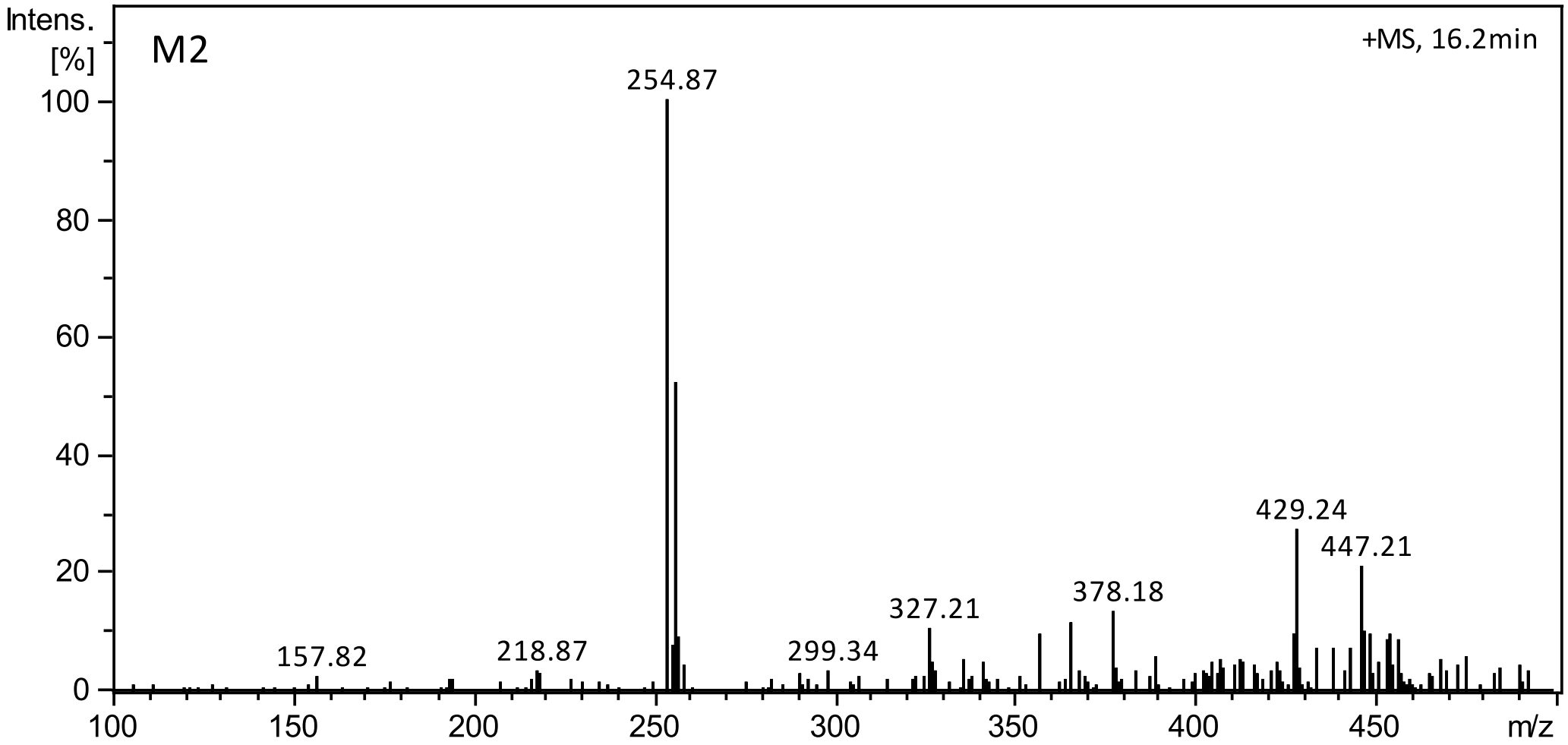

IMZ MS2
+MS2(298.00), 17.9min
Intens. [%]
100
80
60
40
20
0
100
150
200
250
300
350
m/z
254.89
200.81
172.80
158.81
175.86
296.96
-42
-68
-28
-68
-28 CO
-28 CO
or
[M+H]+ 297.05 Da

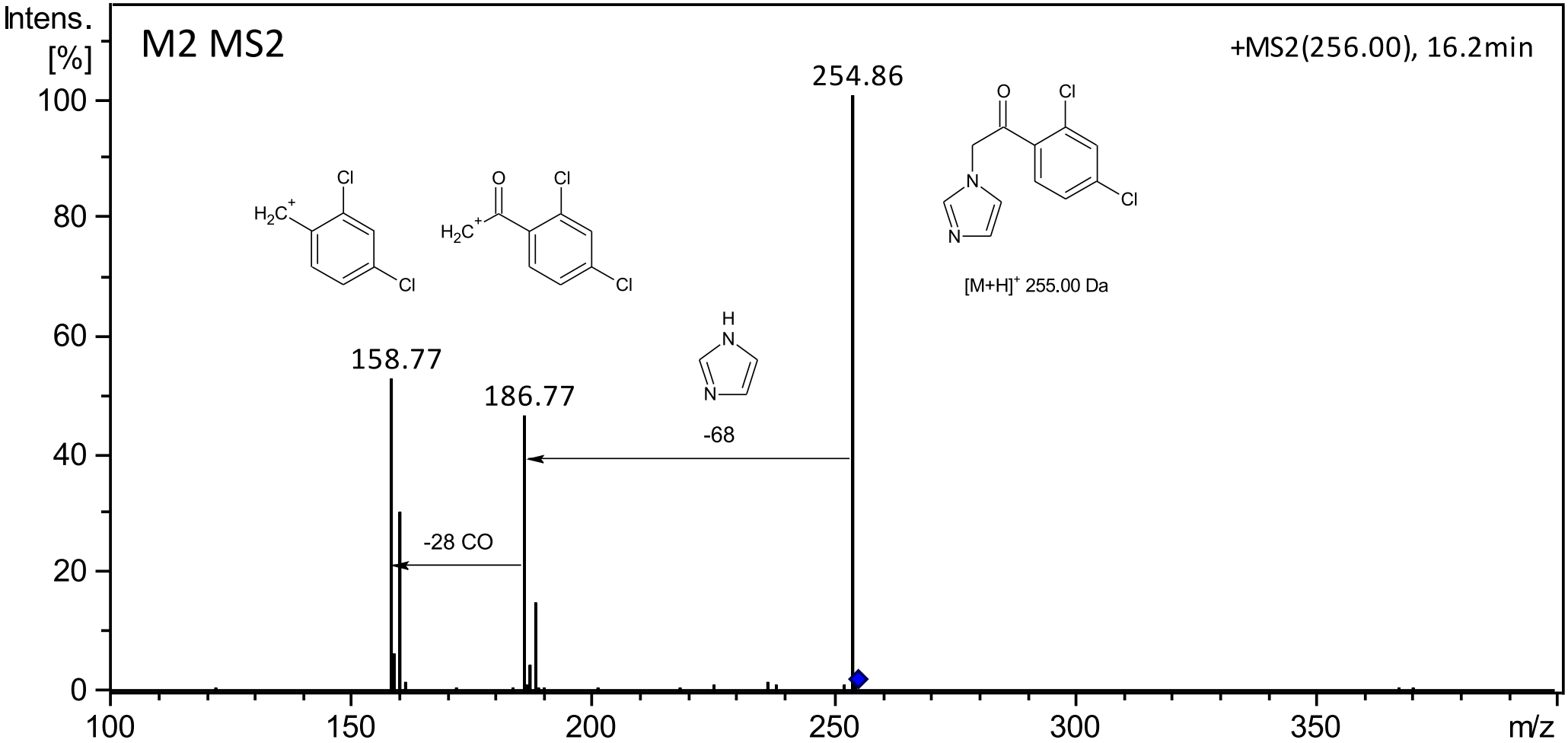

Intens.
[%]
IMZ MS3 a
+MS3(298.00->256.00), 17.9min
254.87
158.80
186.77
-68
-28 CO
m/z
100
80
60
40
20
0
100
150
200
250
300
350

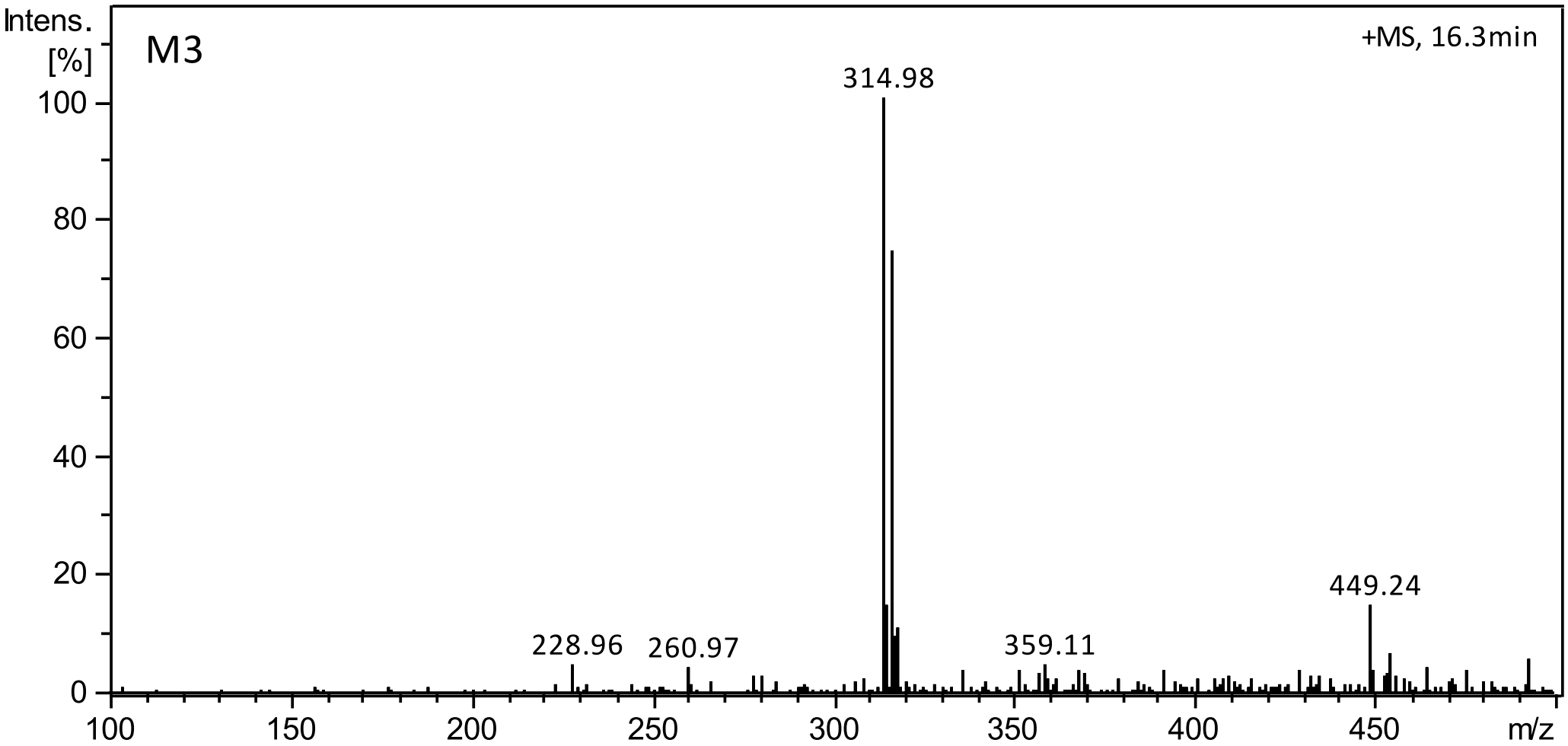

Intens.
[%]
IMZ MS3 b
+MS3(298.00->202.00), 17.9min
172.82
200.80
-28 CO
or
m/z
100
80
60
40
20
0
100
150
200
250
300
350

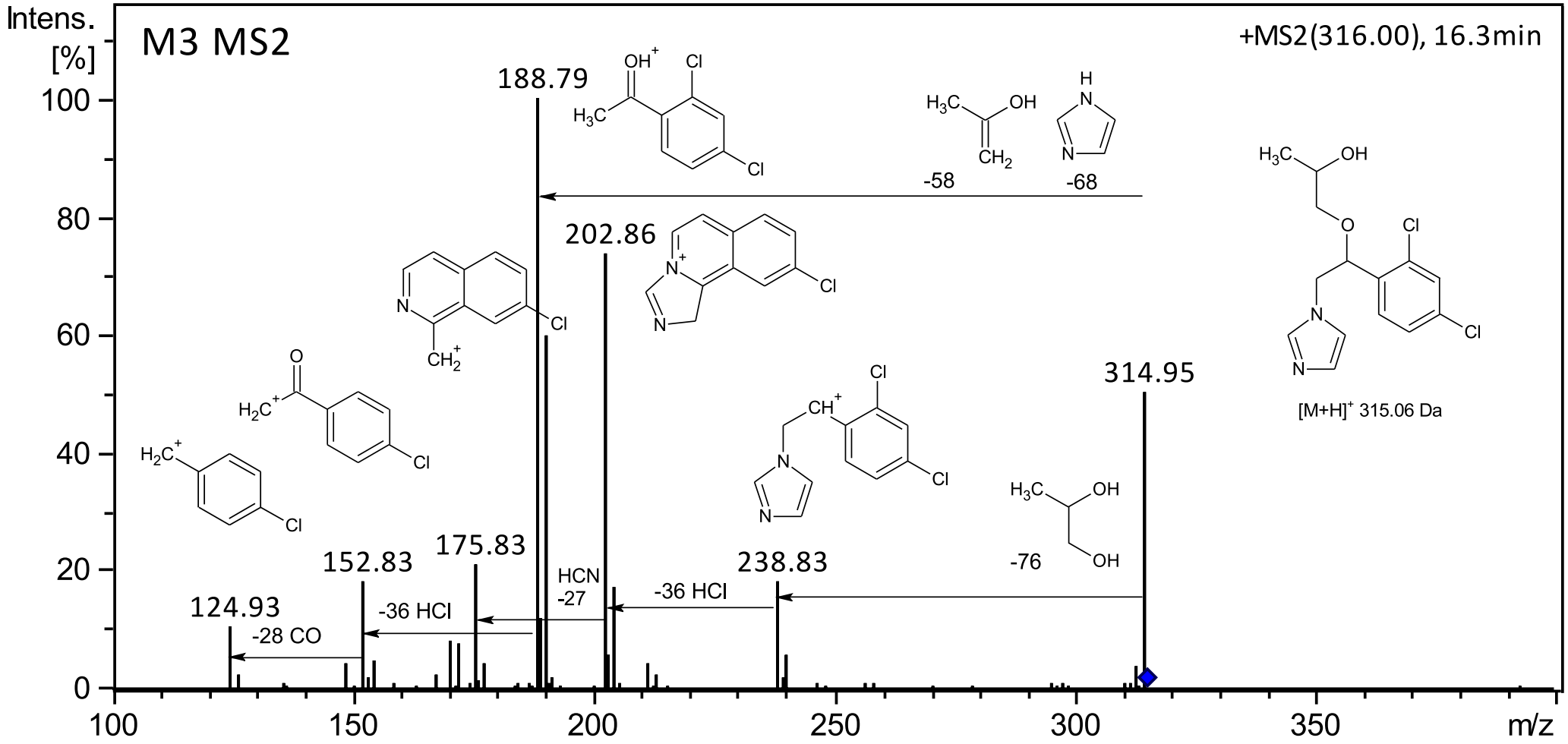

Intens.
[%]
M1
+MS, 15.9min
256.86
378.16
100
80
60
40
20
0
100
150
200
250
300
350
400
450
m/z

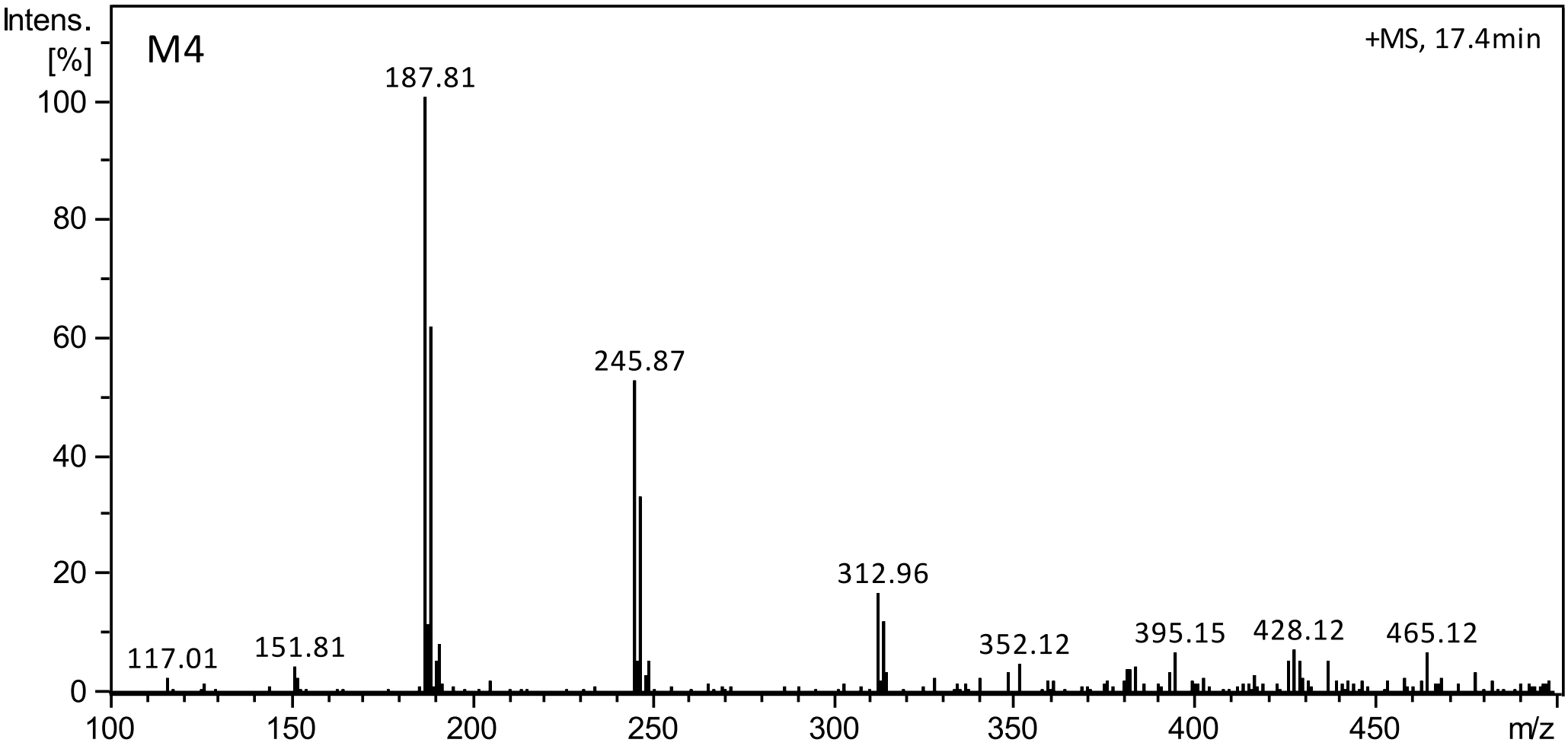

M1 MS2
+MS2(258.00), 15.9min
Intens. [%]
100
80
60
40
20
0
100
150
200
250
300
350
m/z
260.85
188.78
152.81
124.91
-68
-36 HCl
-28 CO
[M+H]+ 257.02 Da

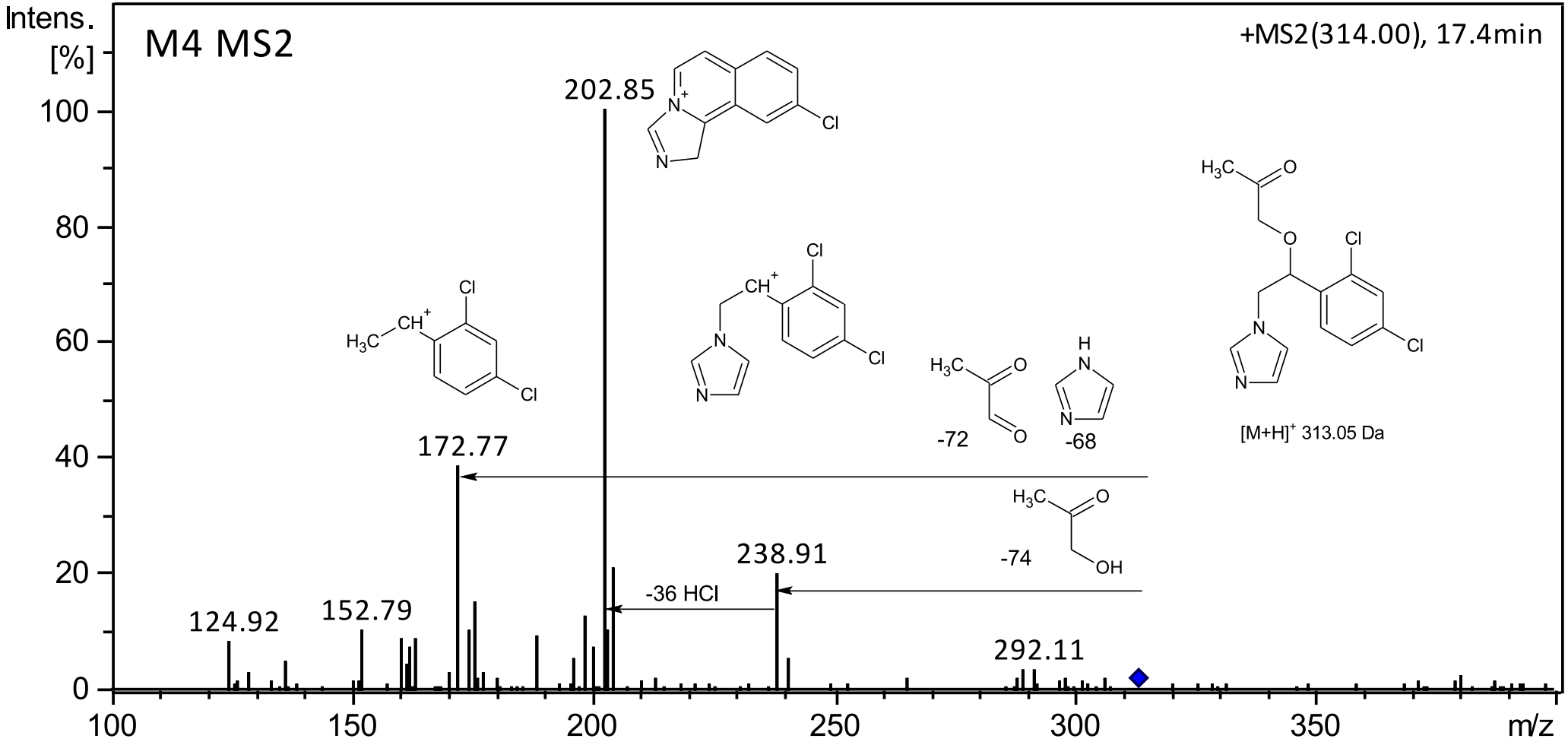

Intens.
[%]
M2
+MS, 16.2min
254.87
429.24
447.21
378.18
327.21
157.82
218.87
299.34
100
80
60
40
20
0
100
150
200
250
300
350
400
450
m/z

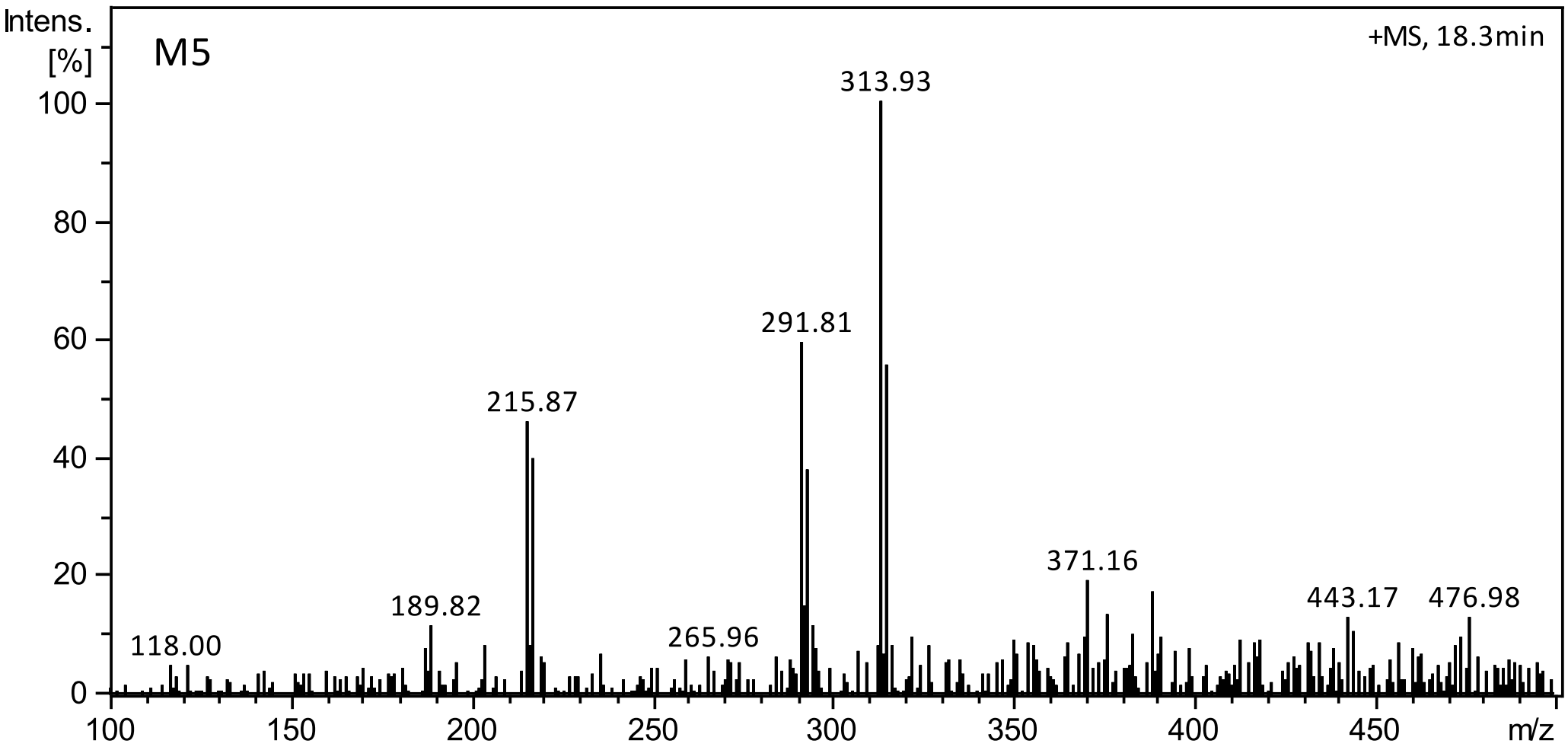

M2 MS2
+MS2(256.00), 16.2min
Intens.
[%]
100
80
60
40
20
0
100
150
200
250
300
350
m/z
254.86
158.77
186.77
-68
-28 CO
[M+H]+ 255.00 Da

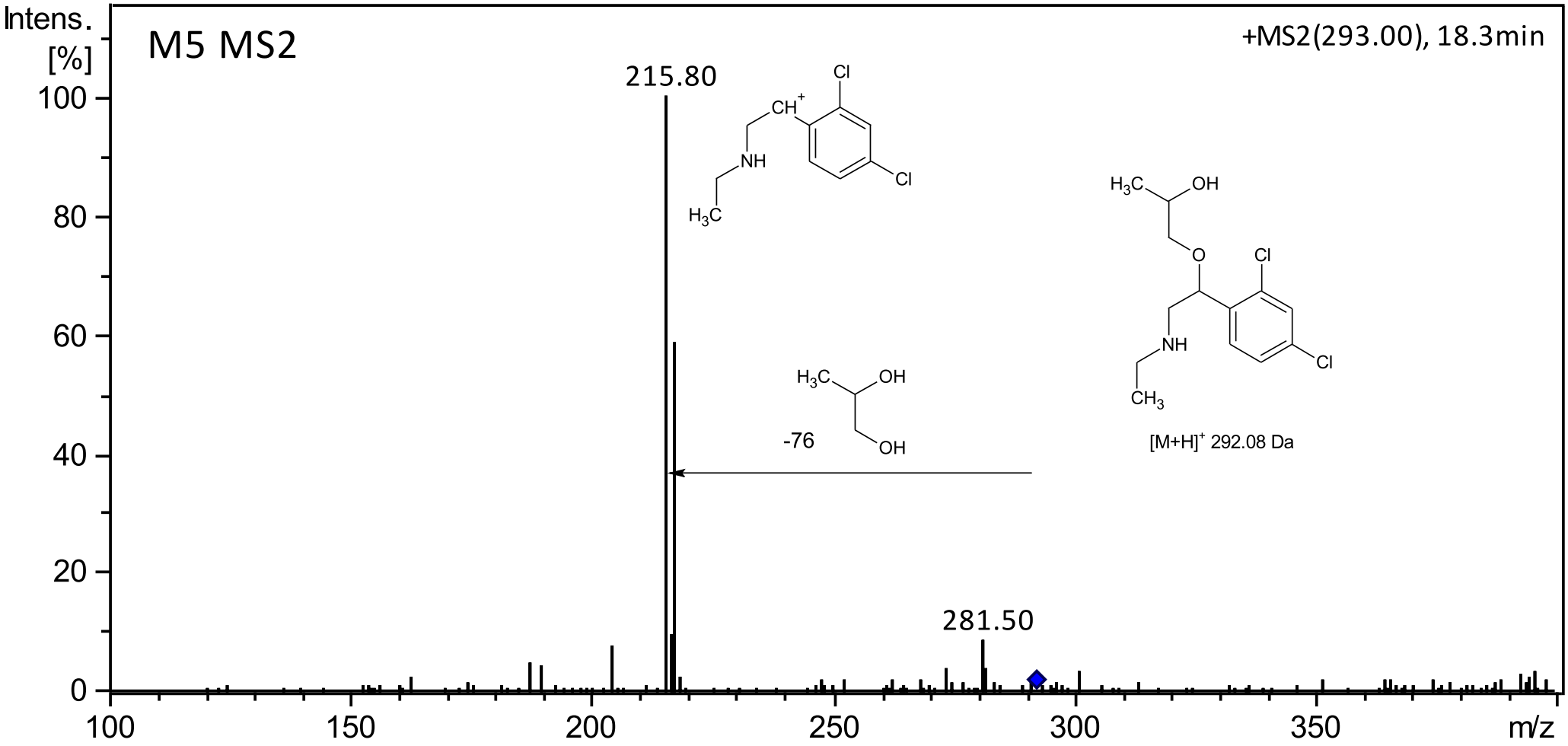

Intens.
[%]
M3
+MS, 16.3min
314.98
449.24
228.96
260.97
359.11
100
80
60
40
20
0
100
150
200
250
300
350
400
450
m/z

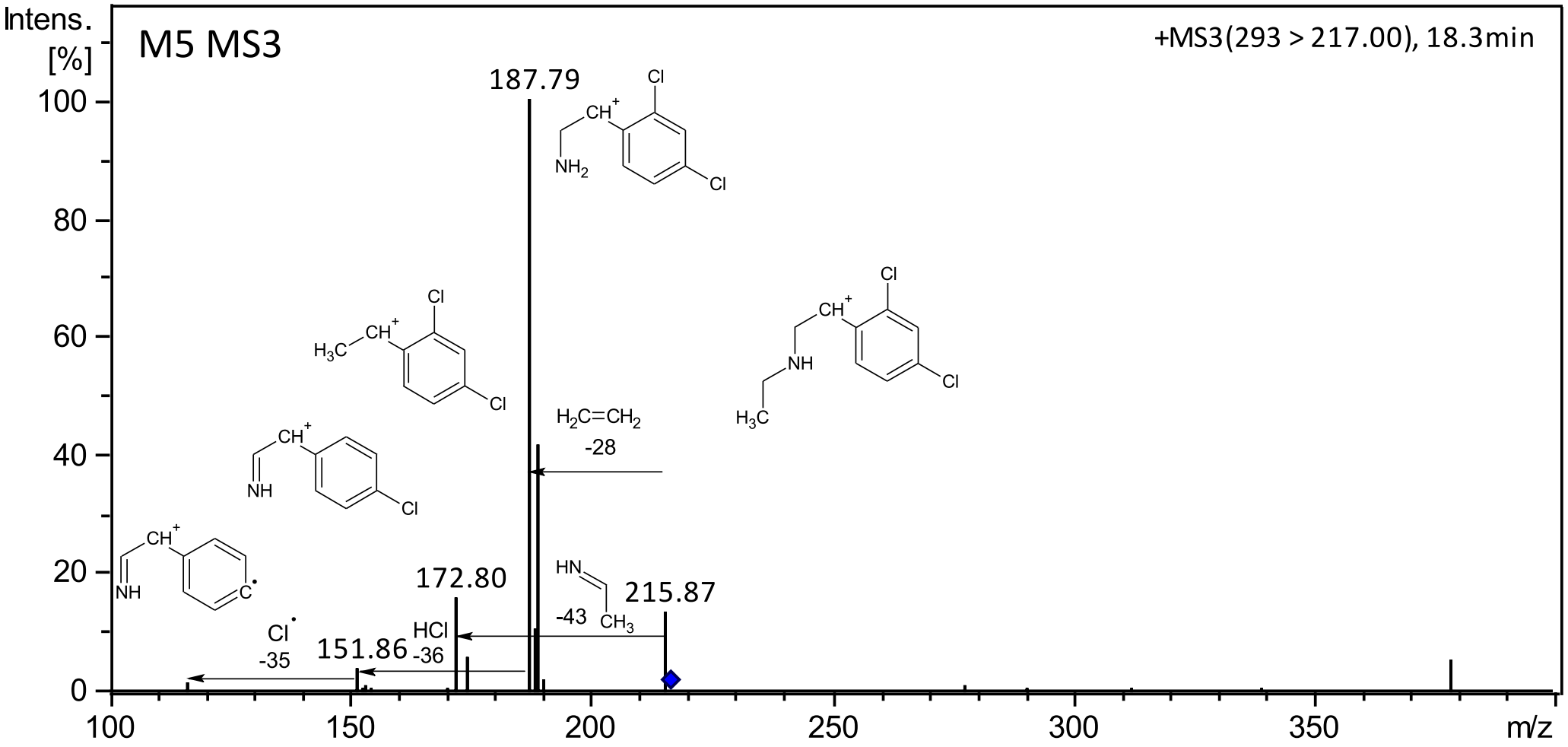

M3 MS2
+MS2(316.00), 16.3min
Intens. [%]
188.79
202.86
314.95
238.83
175.83
152.83
124.93
-58
-68
-76
HCN -27
-36 HCl
-36 HCl
-28 CO
[M+H]+ 315.06 Da
m/z

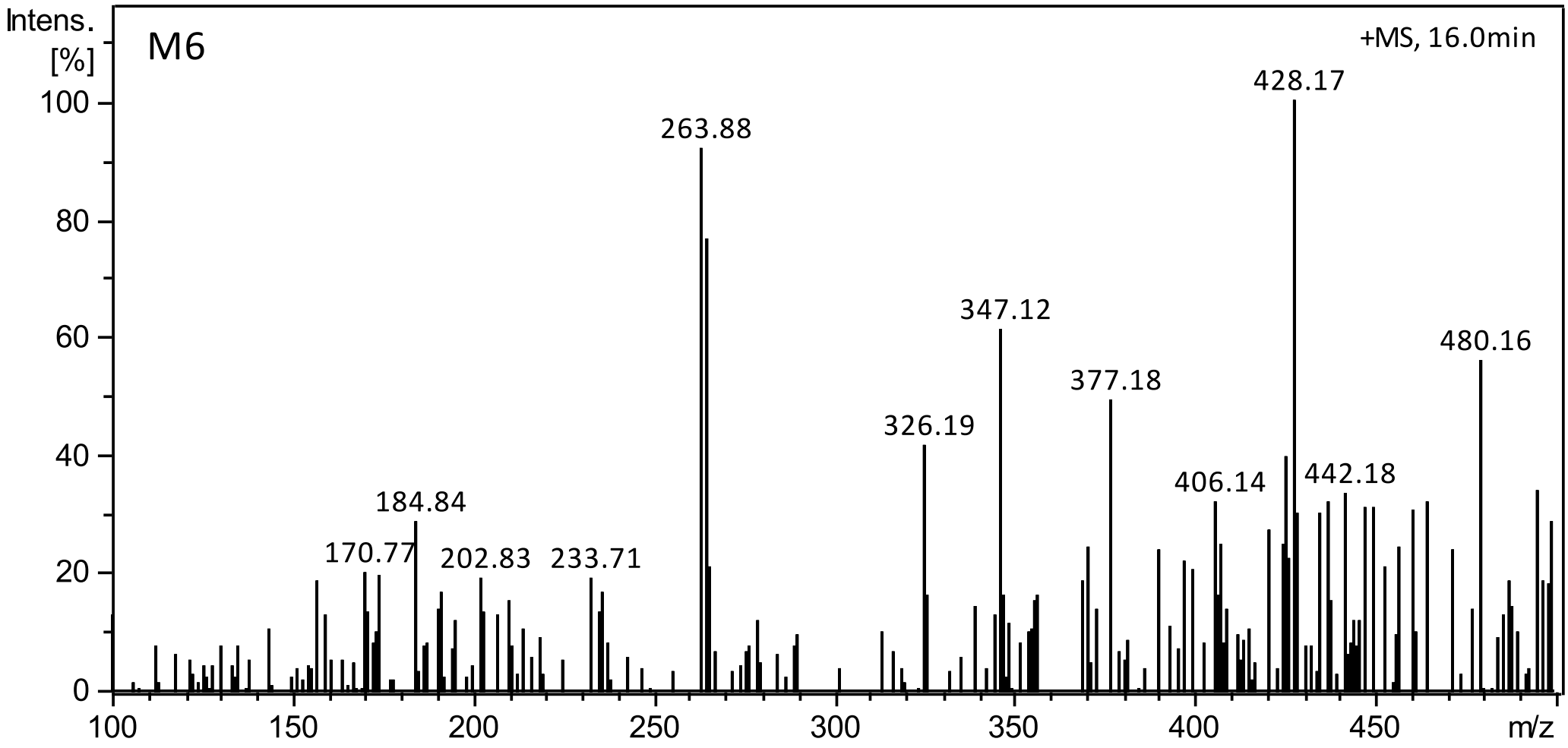

Intens.
[%]
M4
+MS, 17.4min
187.81
245.87
312.96
117.01
151.81
352.12
395.15
428.12
465.12
100
80
60
40
20
0
100
150
200
250
300
350
400
450
m/z

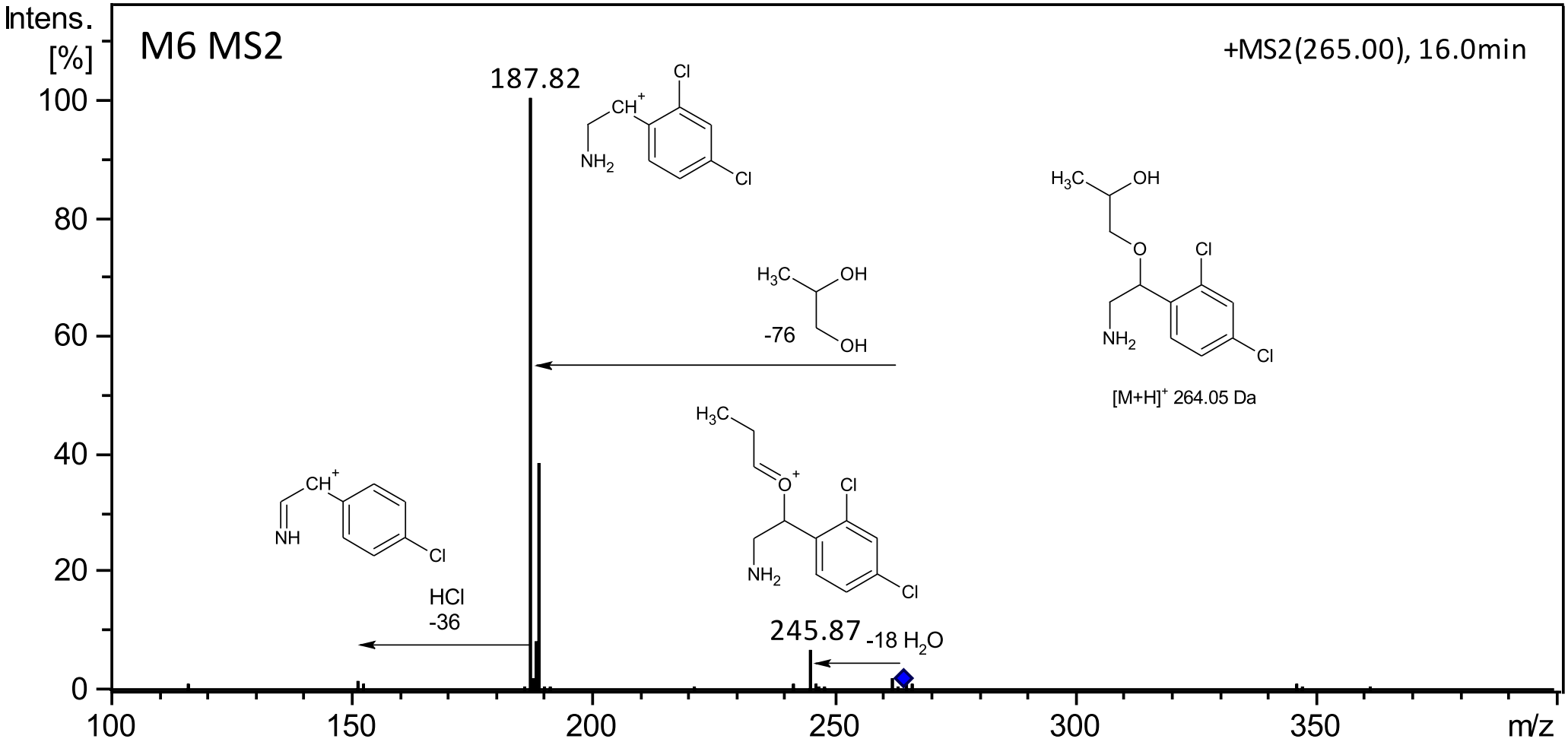

M4 MS2
+MS2(314.00), 17.4min
Intens. [%]
100
80
60
40
20
0
100
150
200
250
300
350
m/z
202.85
172.77
238.91
124.92
152.79
292.11
-36 HCl
-72
-68
-74
[M+H]+ 313.05 Da

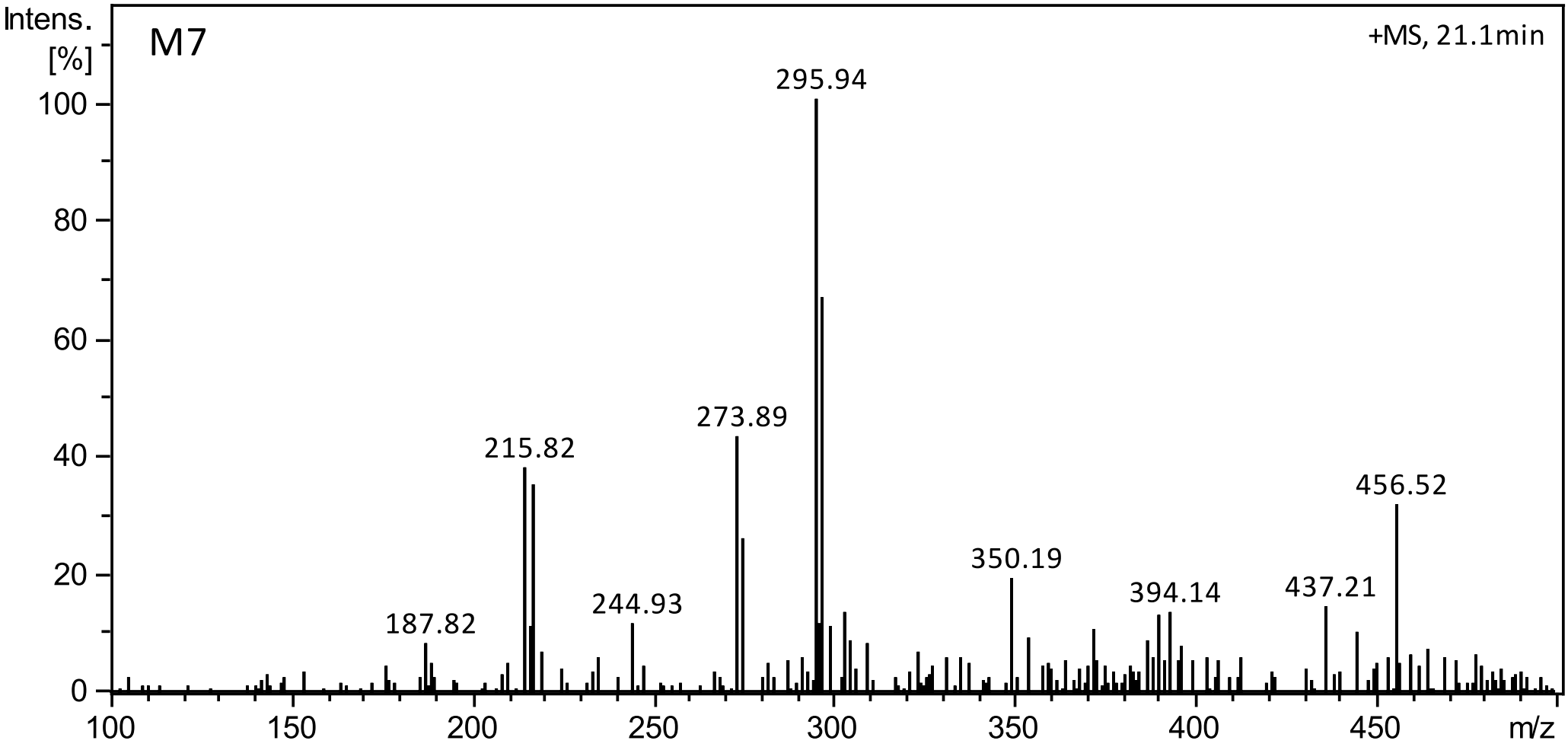

Intens.
[%]
M5
+MS, 18.3min
313.93
291.81
215.87
371.16
443.17
476.98
189.82
265.96
118.00
100
80
60
40
20
0
100
150
200
250
300
350
400
450
m/z

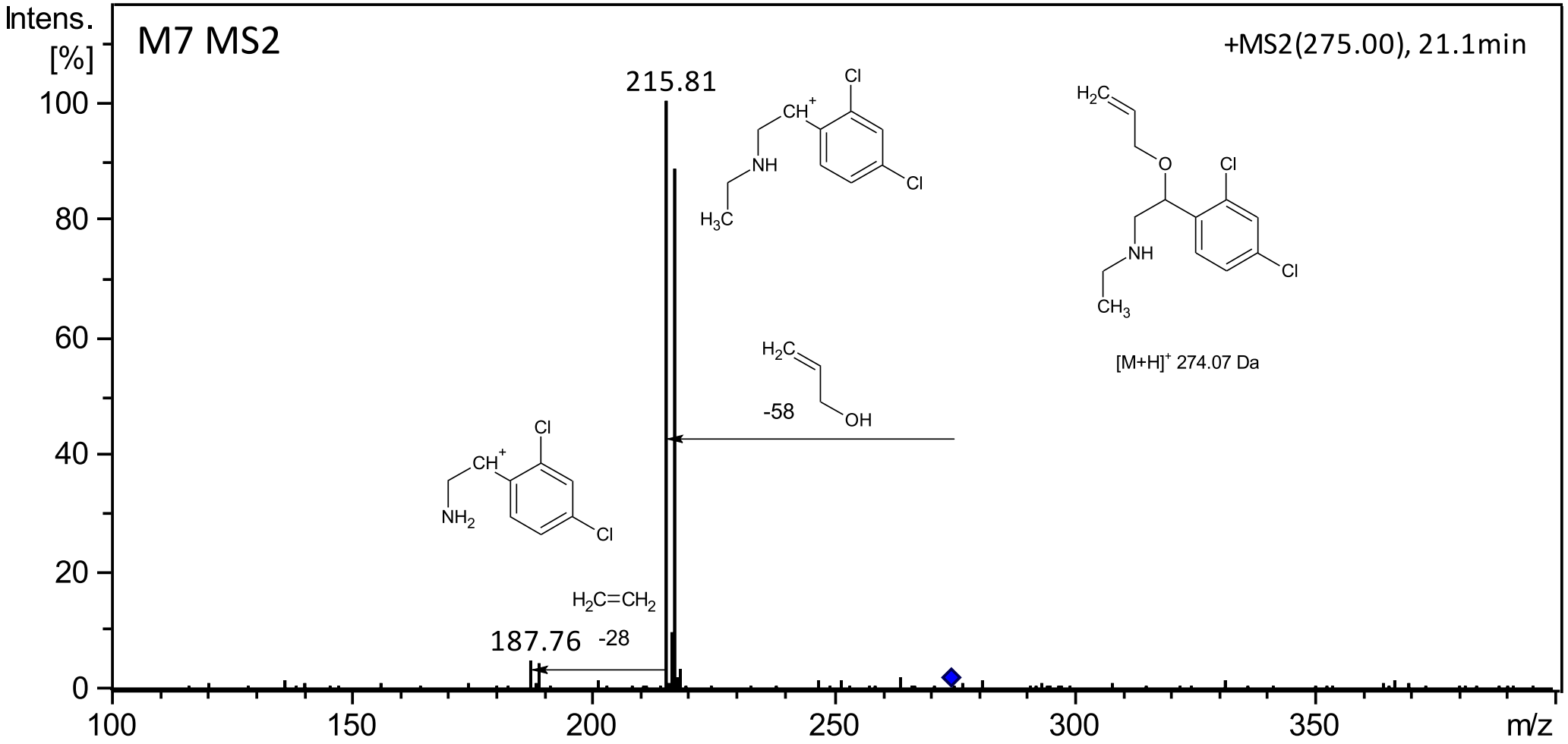

Intens.
[%]
M5 MS2
+MS2(293.00), 18.3min
215.80
281.50
-76
[M+H]+ 292.08 Da
100
80
60
40
20
0
100
150
200
250
300
350
m/z

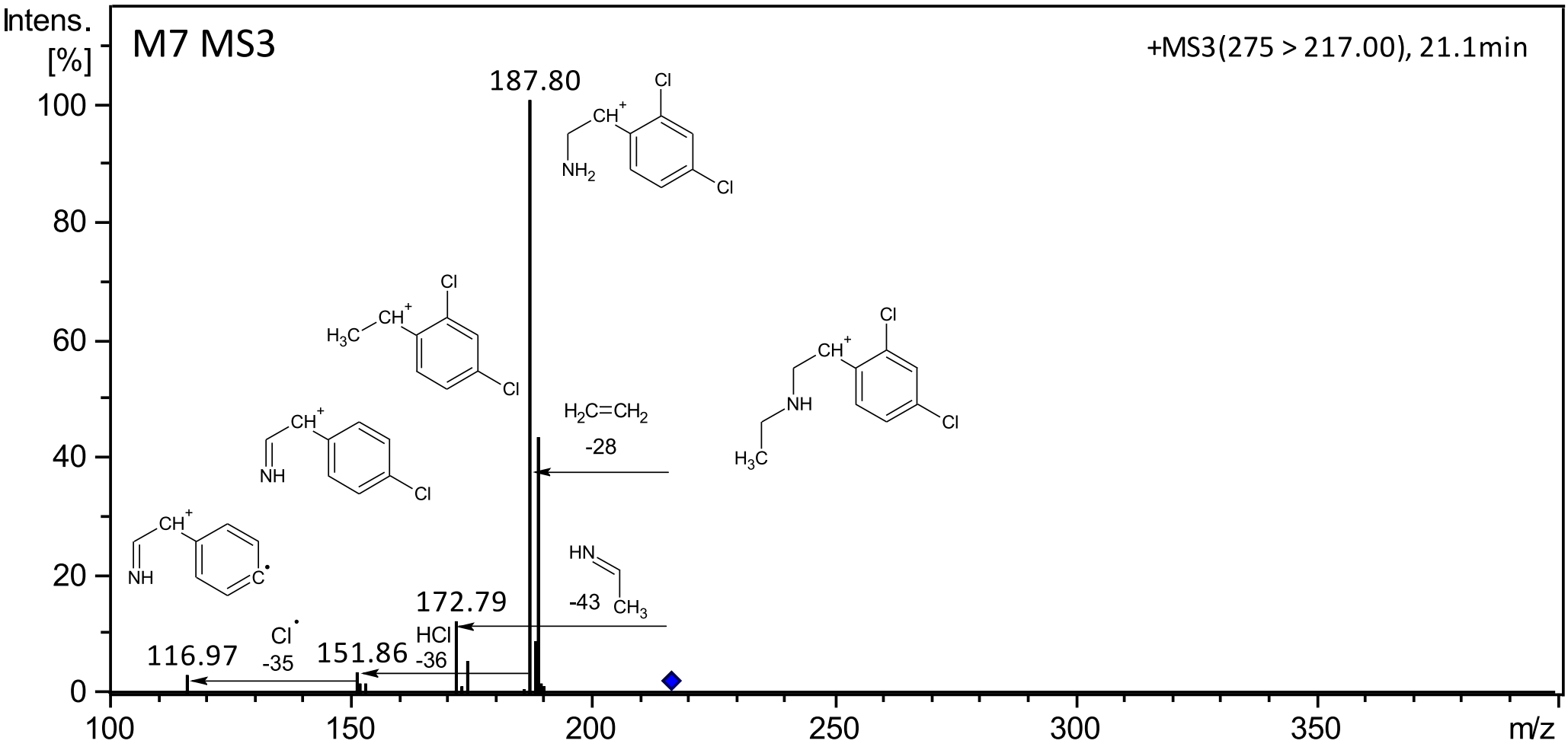

M5 MS3
+MS3(293 > 217.00), 18.3min
Intens. [%]
100
80
60
40
20
0
187.79
172.80
151.86
215.87
H2C=CH2
-28
HCl
-36
Cl•
-35
-43
CH3
m/z
100
150
200
250
300
350

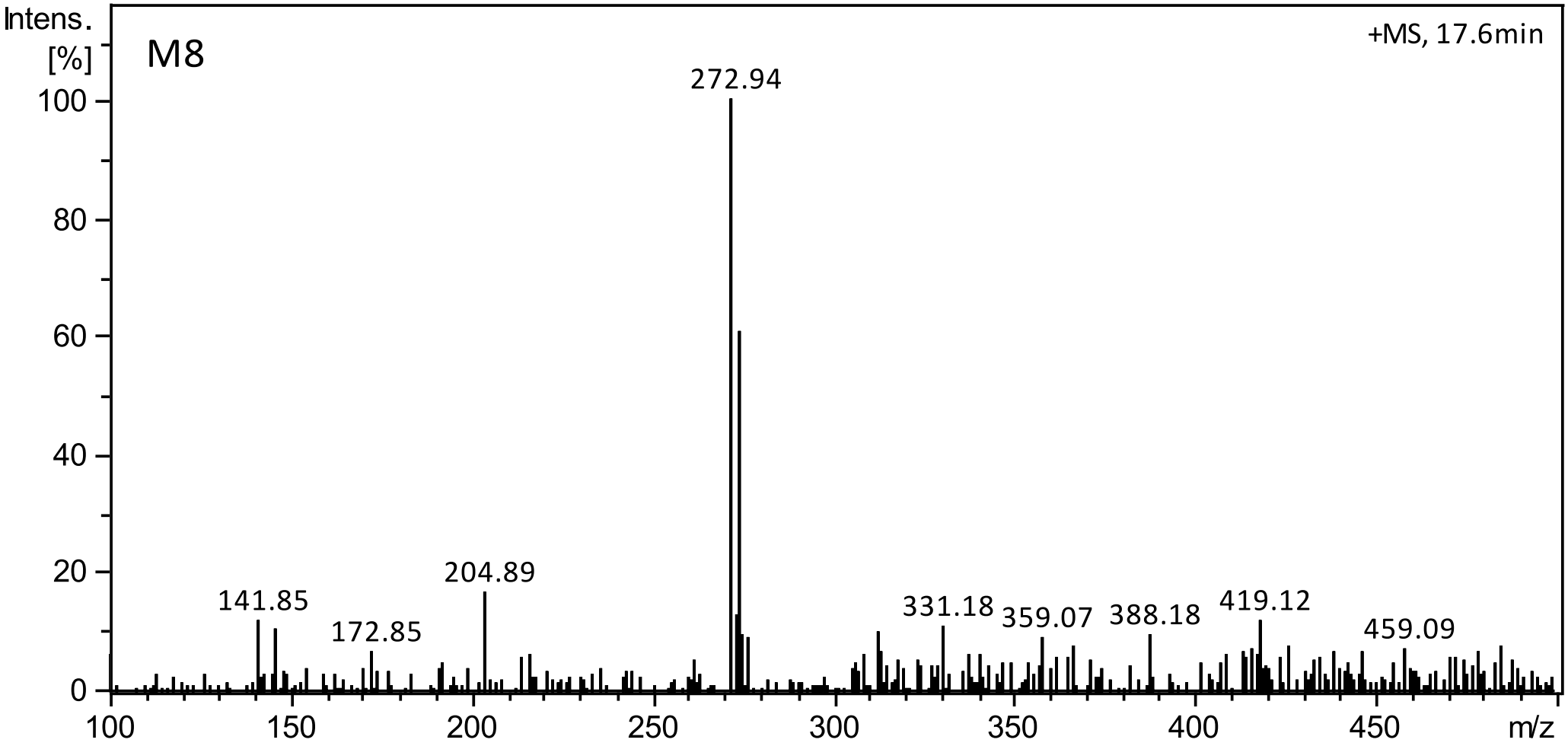

M6
+MS, 16.0min
Intens.
[%]
100
80
60
40
20
0
263.88
428.17
347.12
480.16
377.18
326.19
406.14
442.18
184.84
170.77
202.83
233.71
100
150
200
250
300
350
400
450
m/z

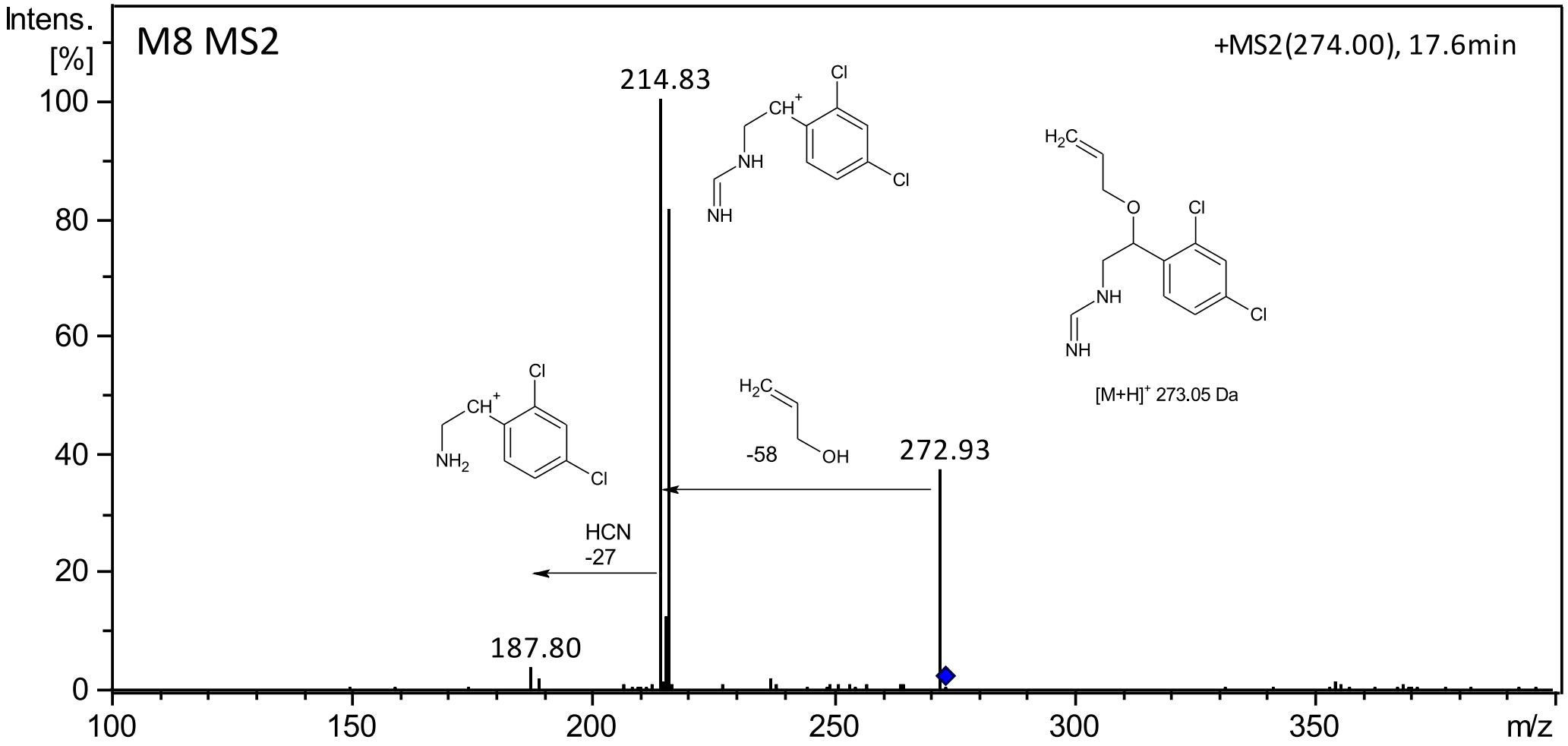

M6 MS2
+MS2(265.00), 16.0min
Intens.
[%]
100
80
60
40
20
0
100
150
200
250
300
350
m/z
187.82
245.87
-18 H2O
HCl
-36
-76
[M+H]+ 264.05 Da

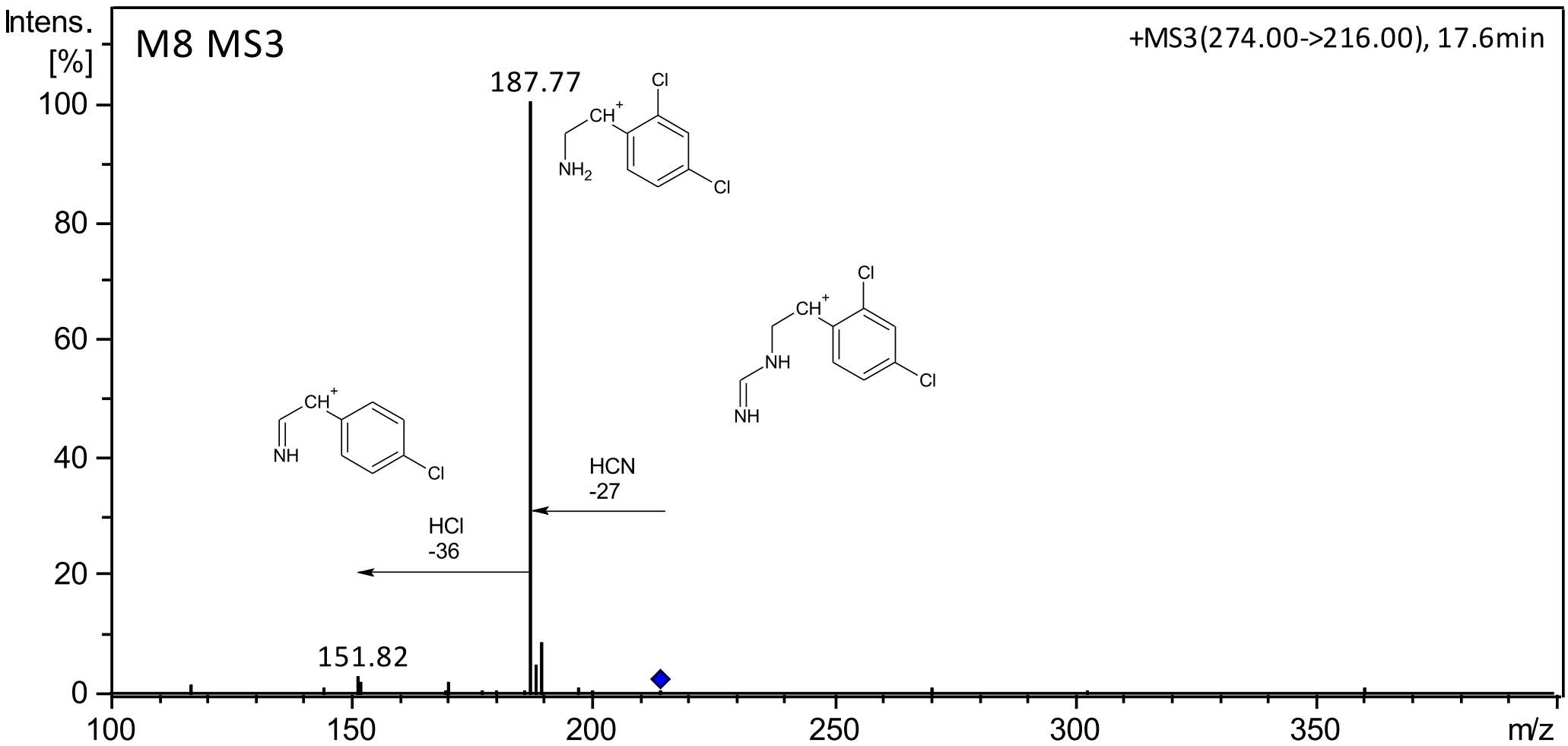

M7
+MS, 21.1min
Intens.
[%]
100
80
60
40
20
0
295.94
273.89
215.82
456.52
350.19
394.14
437.21
244.93
187.82
100
150
200
250
300
350
400
450
m/z

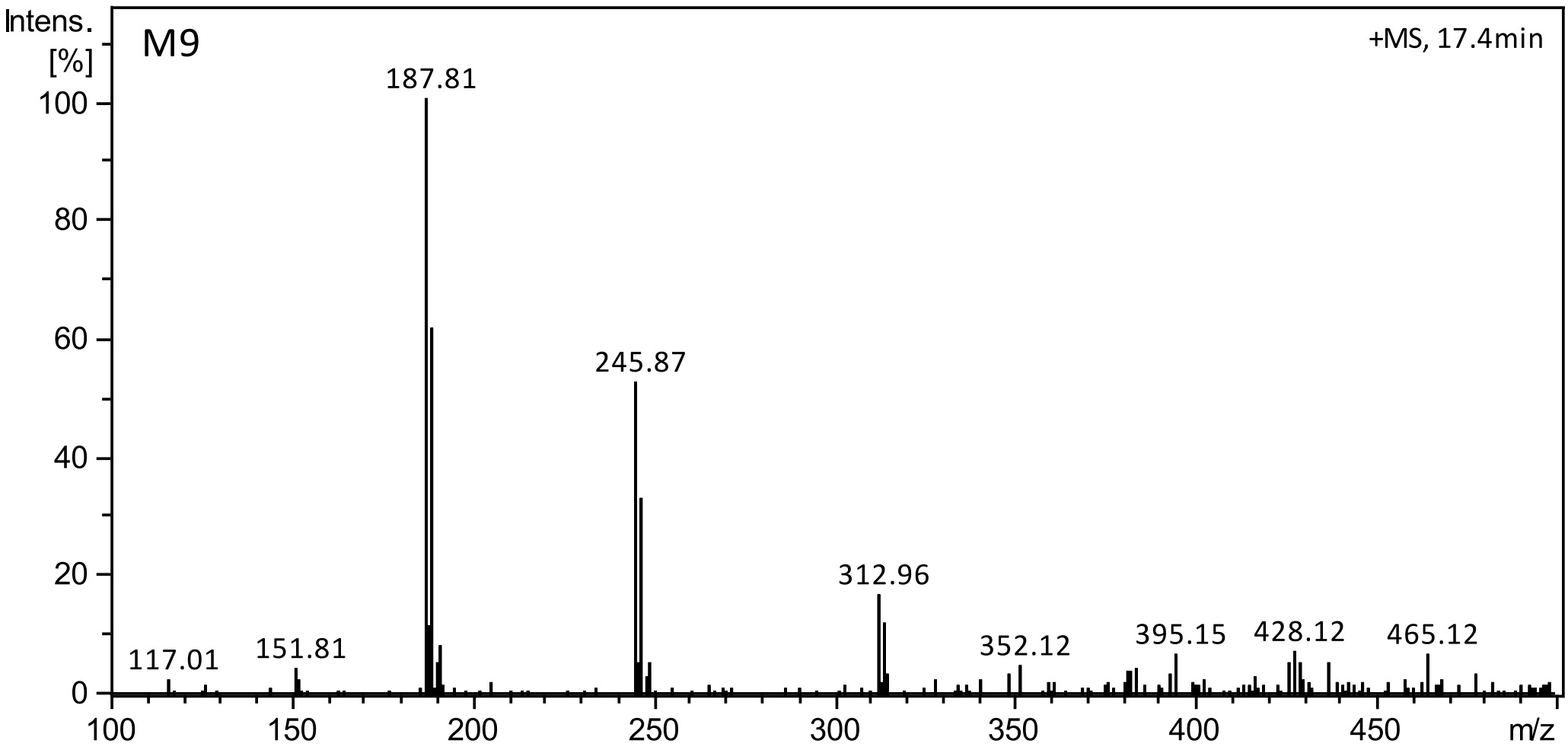

M7 MS2
+MS2(275.00), 21.1min
Intens.
[%]
100
80
60
40
20
0
215.81
187.76
-28
$H_2C{=}CH_2$
-58
$[M+H]^+$ 274.07 Da
100
150
200
250
300
350
m/z

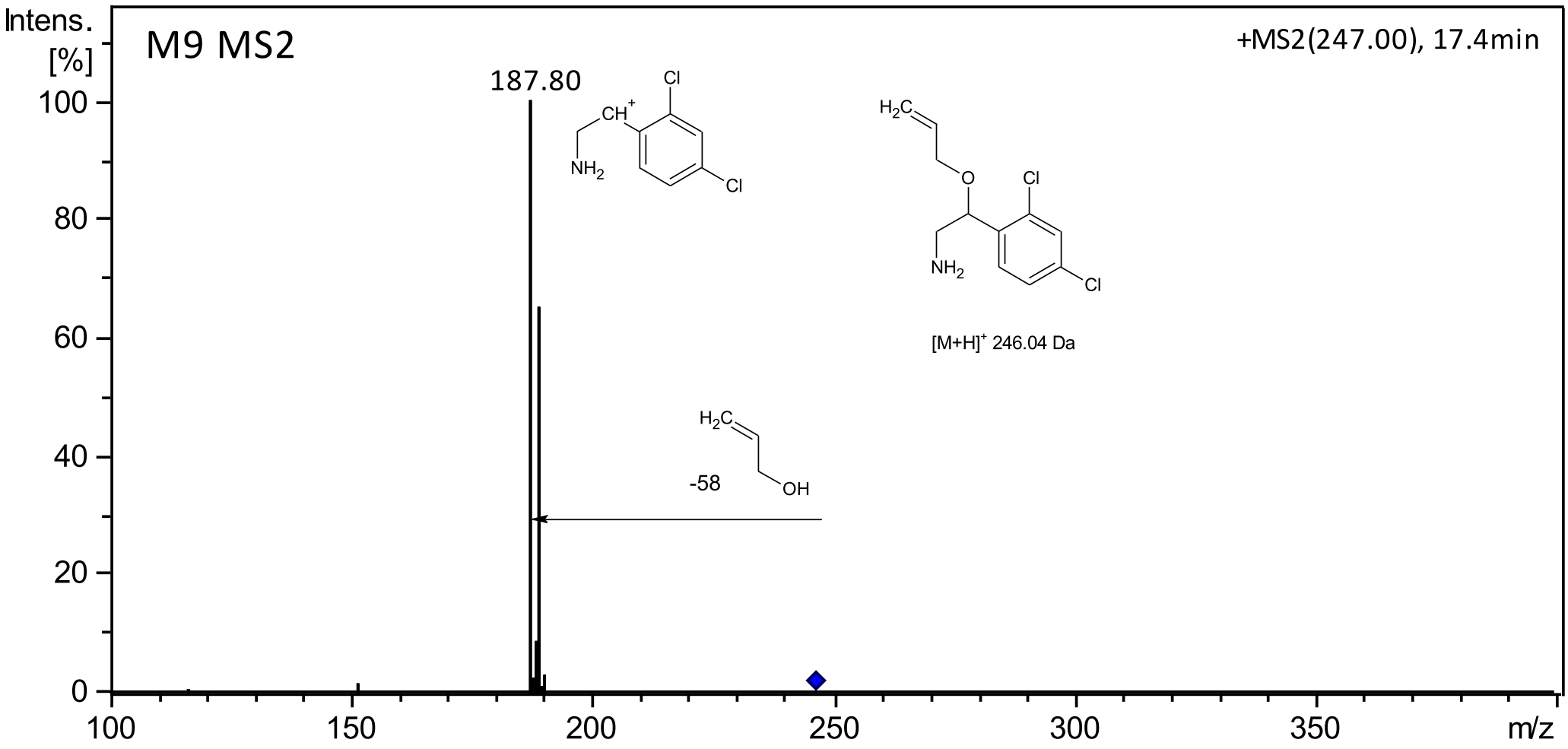

M7 MS3
+MS3(275 > 217.00), 21.1min
Intens.
[%]
100
80
60
40
20
0
187.80
172.79
151.86
116.97
Cl•
-35
HCl
-36
H2C=CH2
-28
HN
CH3
-43
100
150
200
250
300
350
m/z

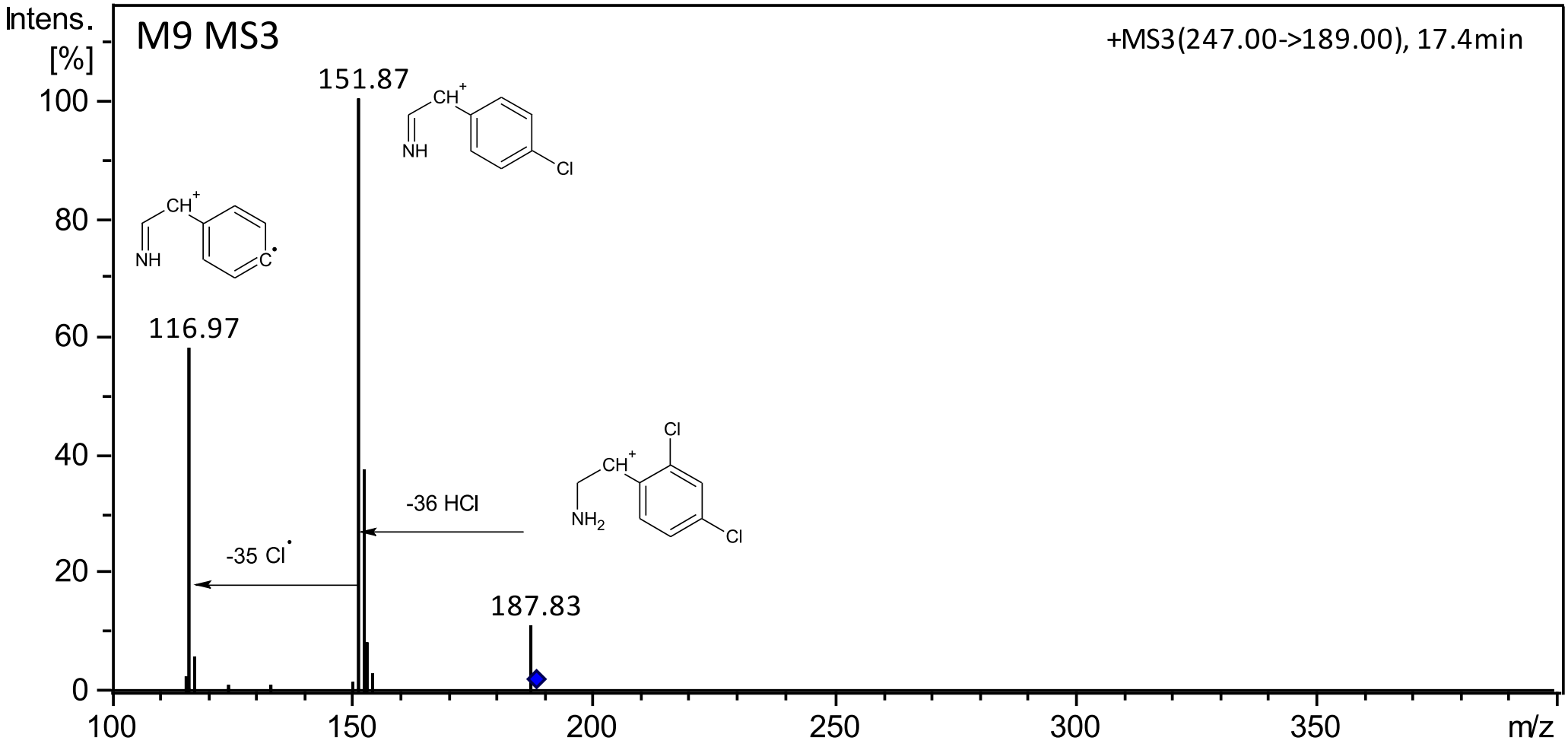

Intens.
[%]
M8
+MS, 17.6min
272.94
204.89
141.85
172.85
331.18
359.07
388.18
419.12
459.09
100
80
60
40
20
0
100
150
200
250
300
350
400
450
m/z

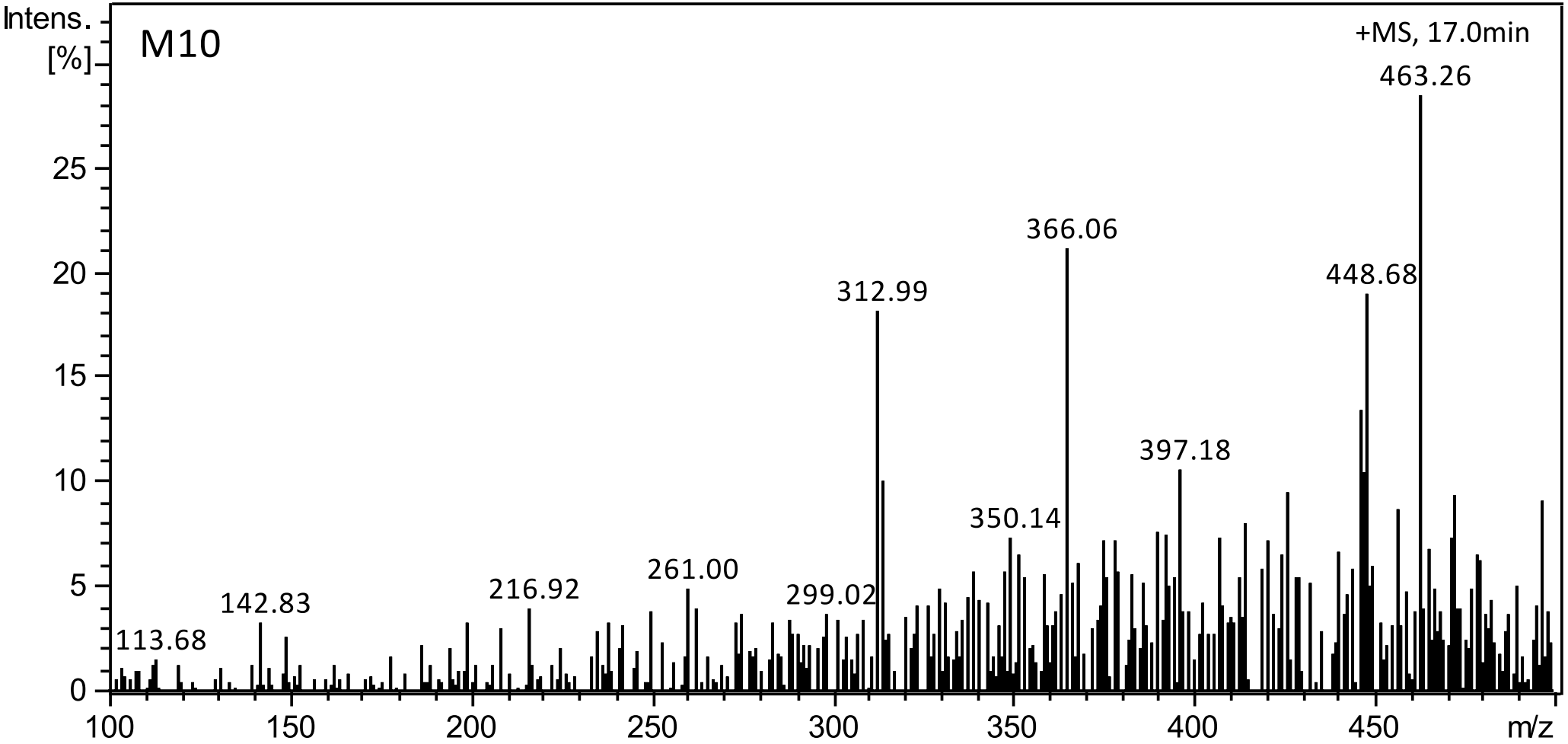

M8 MS2
+MS2(274.00), 17.6min
Intens.
[%]
100
80
60
40
20
0
214.83
272.93
187.80
HCN
-27
-58
[M+H]+ 273.05 Da
100
150
200
250
300
350
m/z

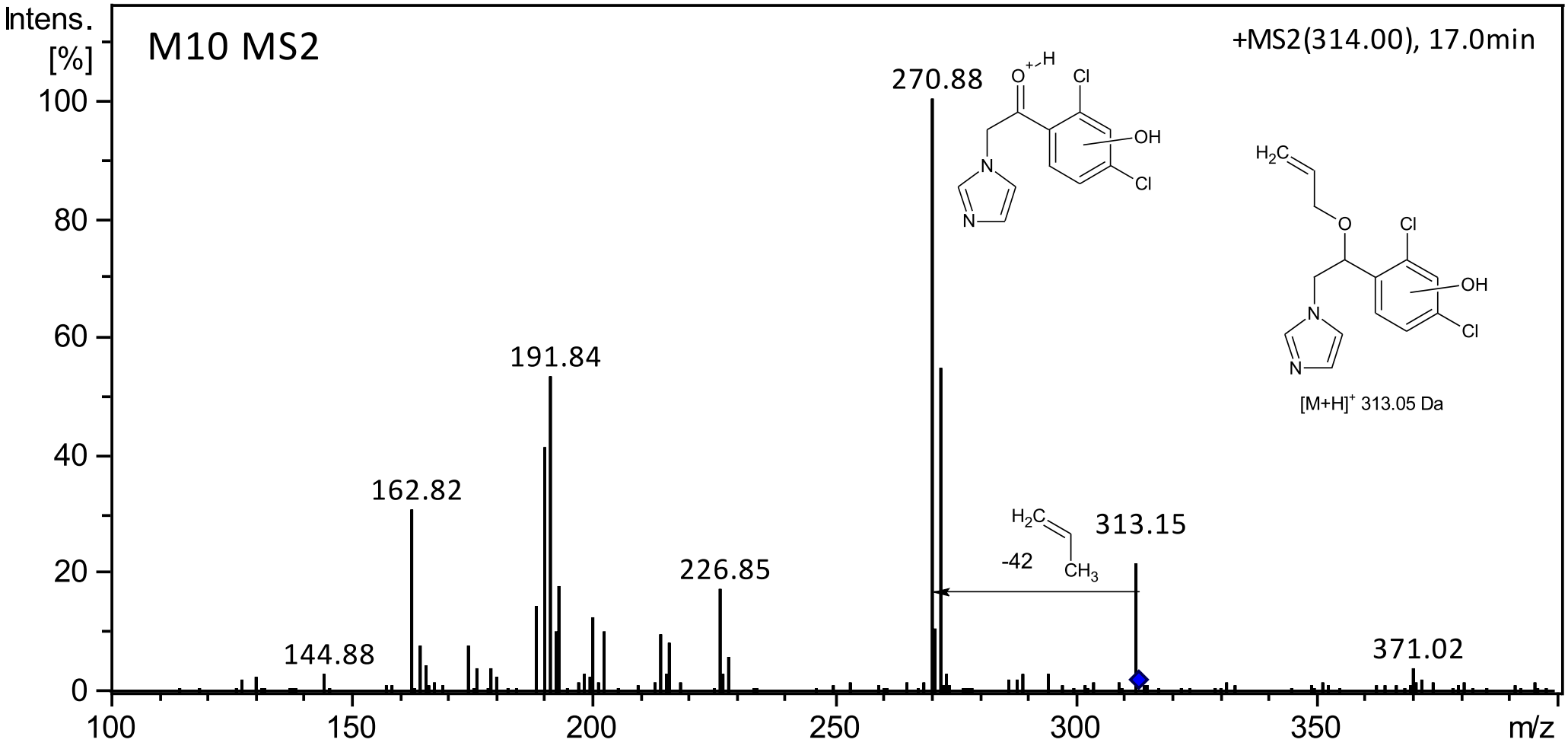

M8 MS3
+MS3(274.00->216.00), 17.6min
Intens.
[%]
100
80
60
40
20
0
187.77
151.82
HCN
-27
HCl
-36
100
150
200
250
300
350
m/z

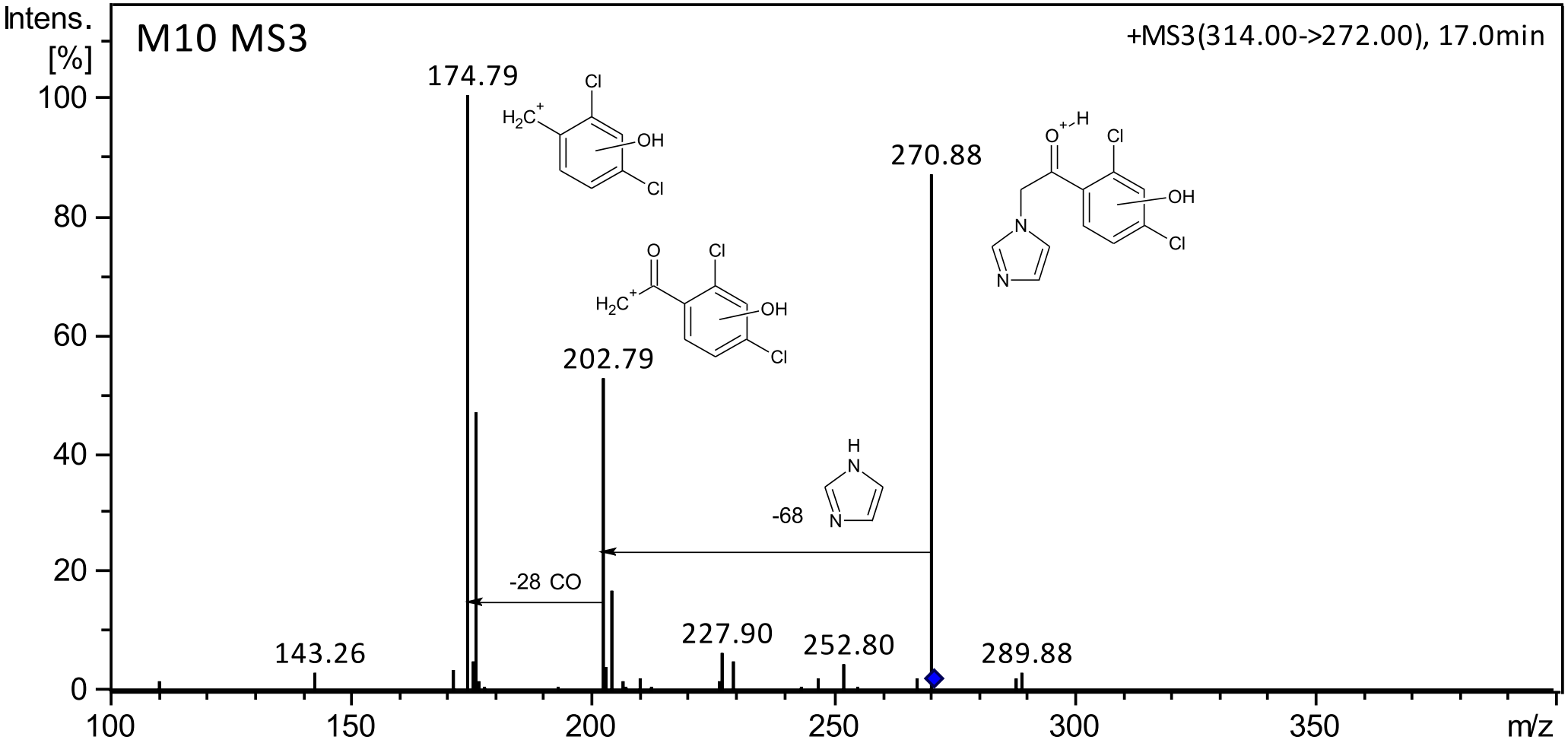

M9
+MS, 17.4min
Intens.
[%]
100
80
60
40
20
0
187.81
245.87
312.96
117.01
151.81
352.12
395.15
428.12
465.12
100
150
200
250
300
350
400
450
m/z

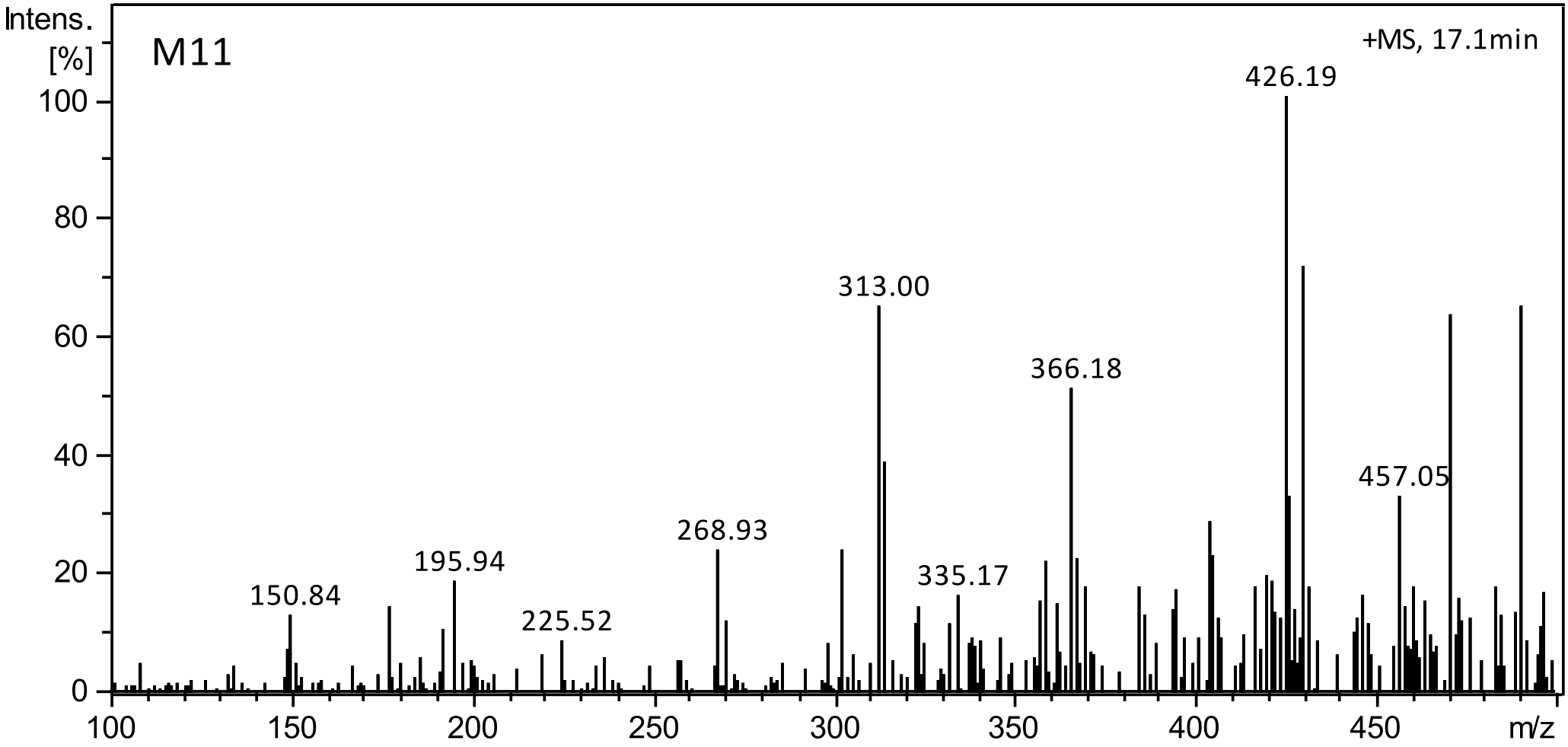

M9 MS2
+MS2(247.00), 17.4min
Intens.
[%]
100
80
60
40
20
0
187.80
CH+
Cl
NH2
Cl
H2C
O
Cl
NH2
Cl
[M+H]+ 246.04 Da
H2C
-58
OH
100
150
200
250
300
350
m/z

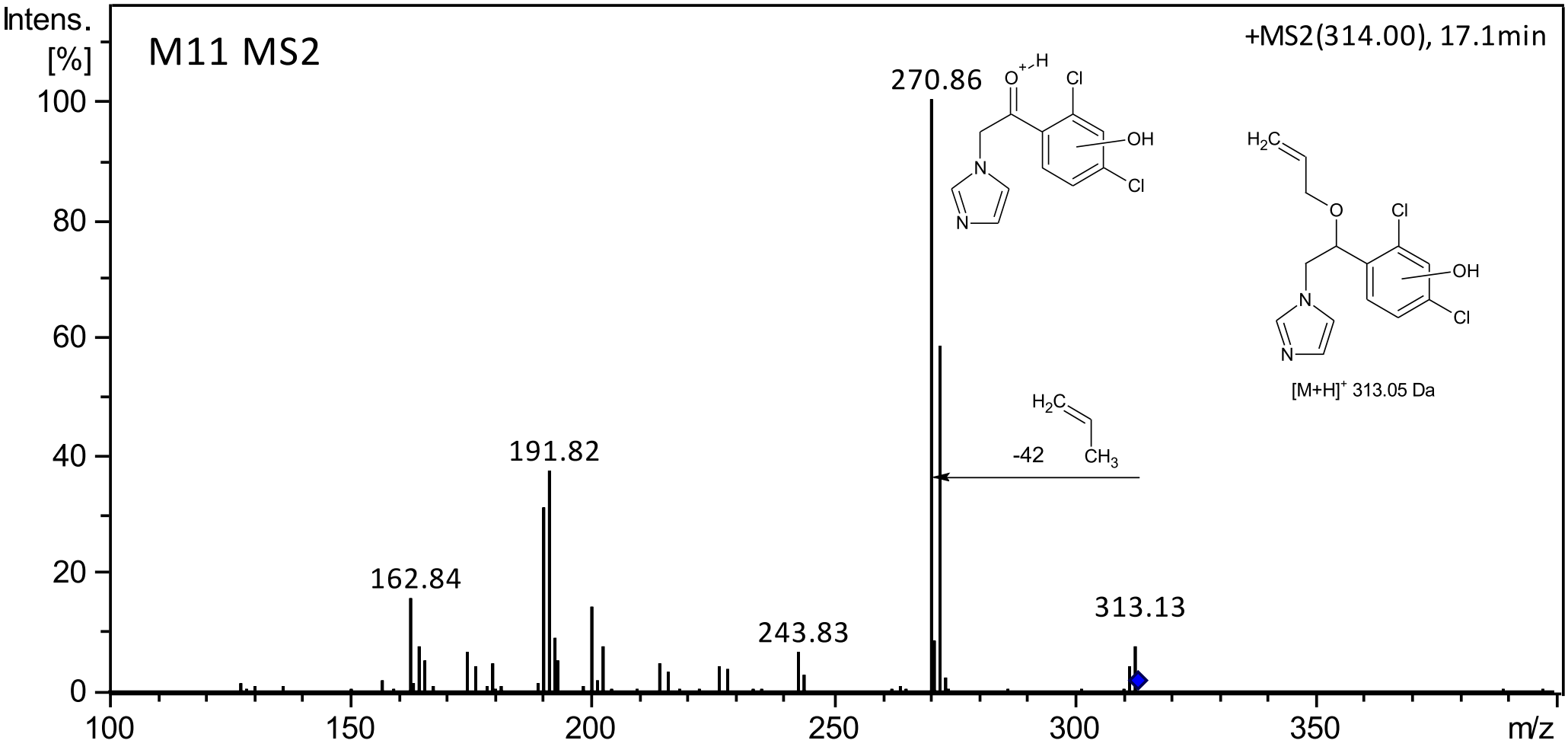

M9 MS3
+MS3(247.00->189.00), 17.4min
Intens.
[%]
100
80
60
40
20
0
151.87
116.97
187.83
-36 HCl
-35 Cl•
CH+
NH
Cl
C•
NH2
100
150
200
250
300
350
m/z

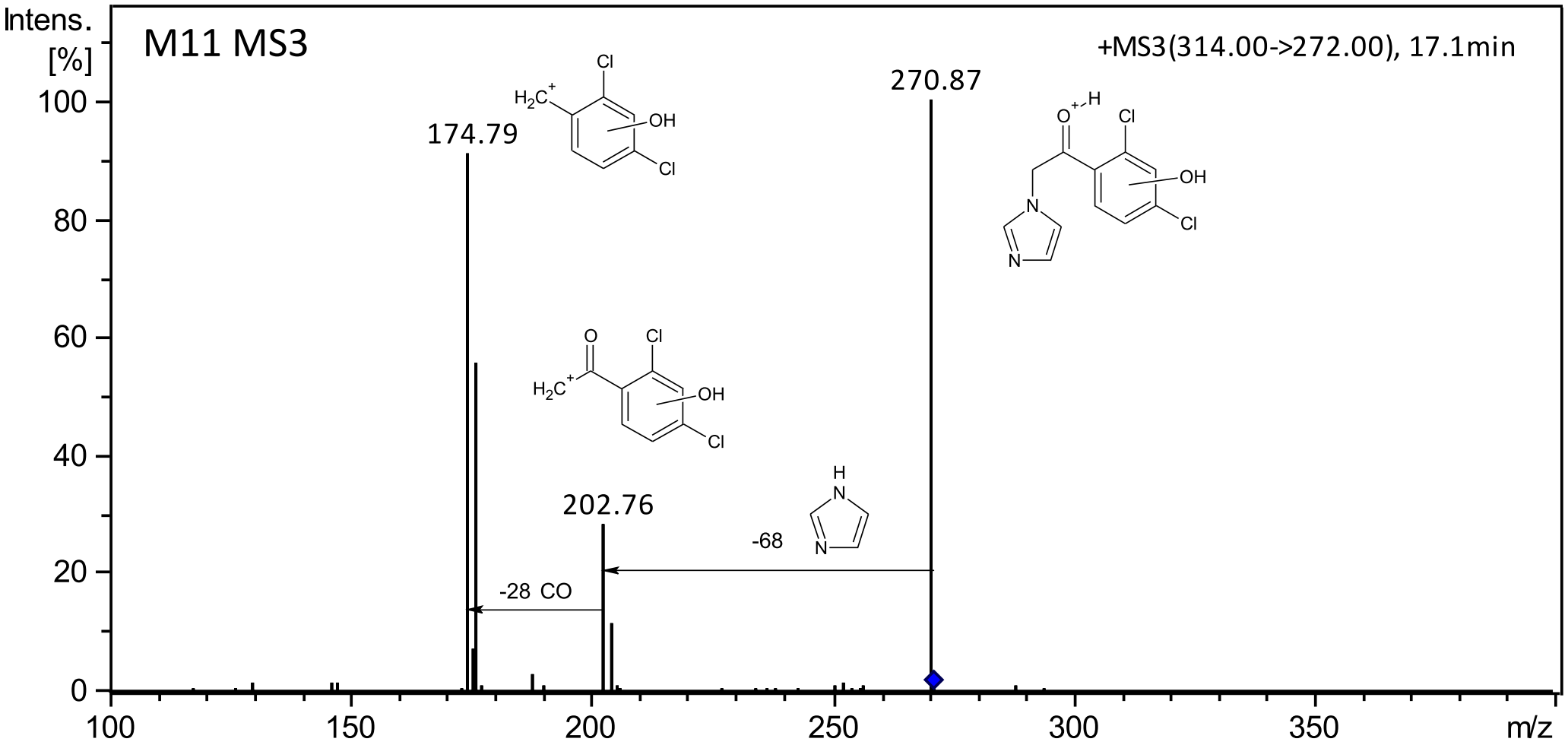

M10
+MS, 17.0min
Intens.
[%]
463.26
366.06
448.68
312.99
397.18
350.14
261.00
216.92
299.02
142.83
113.68
25
20
15
10
5
0
100
150
200
250
300
350
400
450
m/z

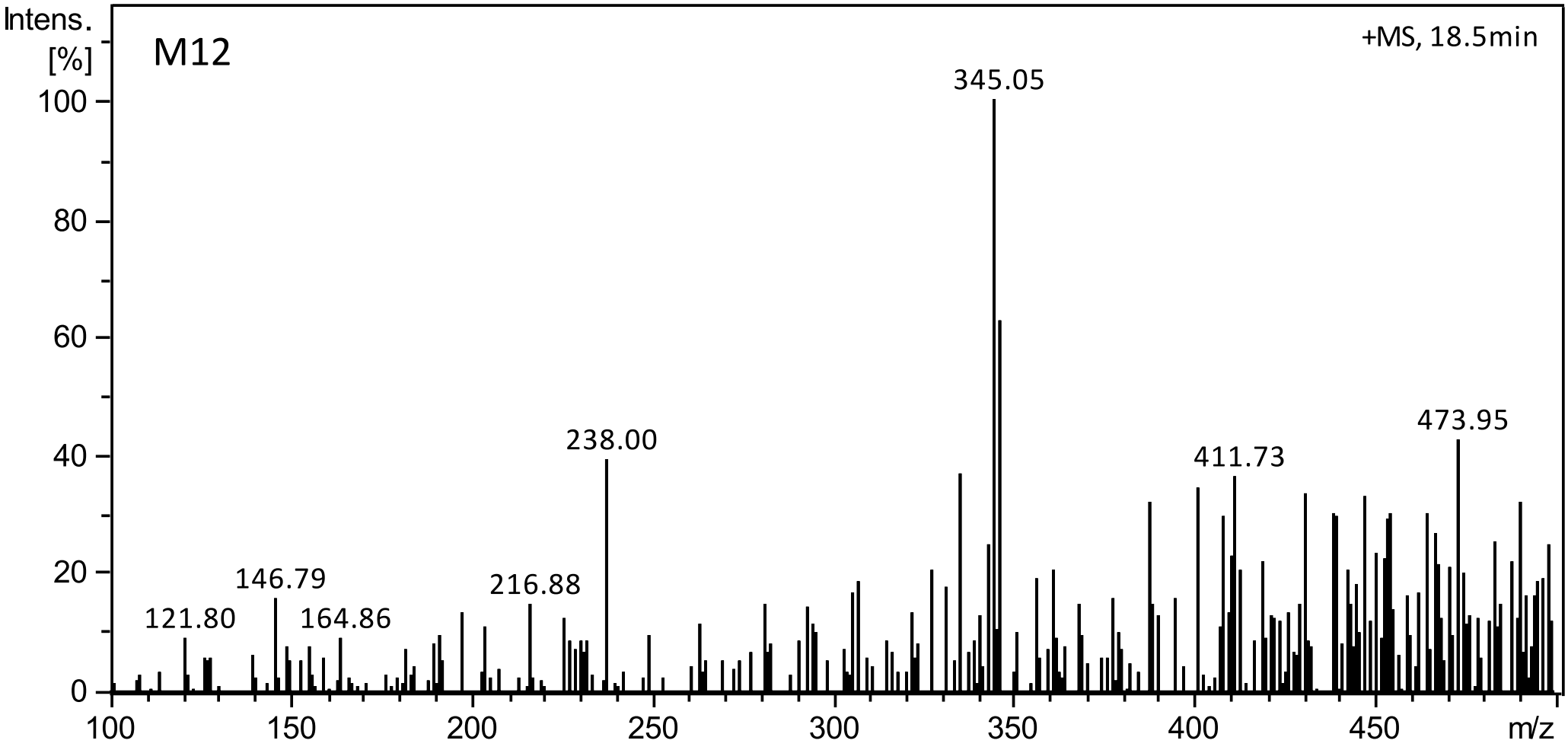

M10 MS2
+MS2(314.00), 17.0min
Intens.
[%]
100
80
60
40
20
0
100
150
200
250
300
350
m/z
270.88
191.84
162.82
226.85
144.88
313.15
371.02
-42
[M+H]+ 313.05 Da

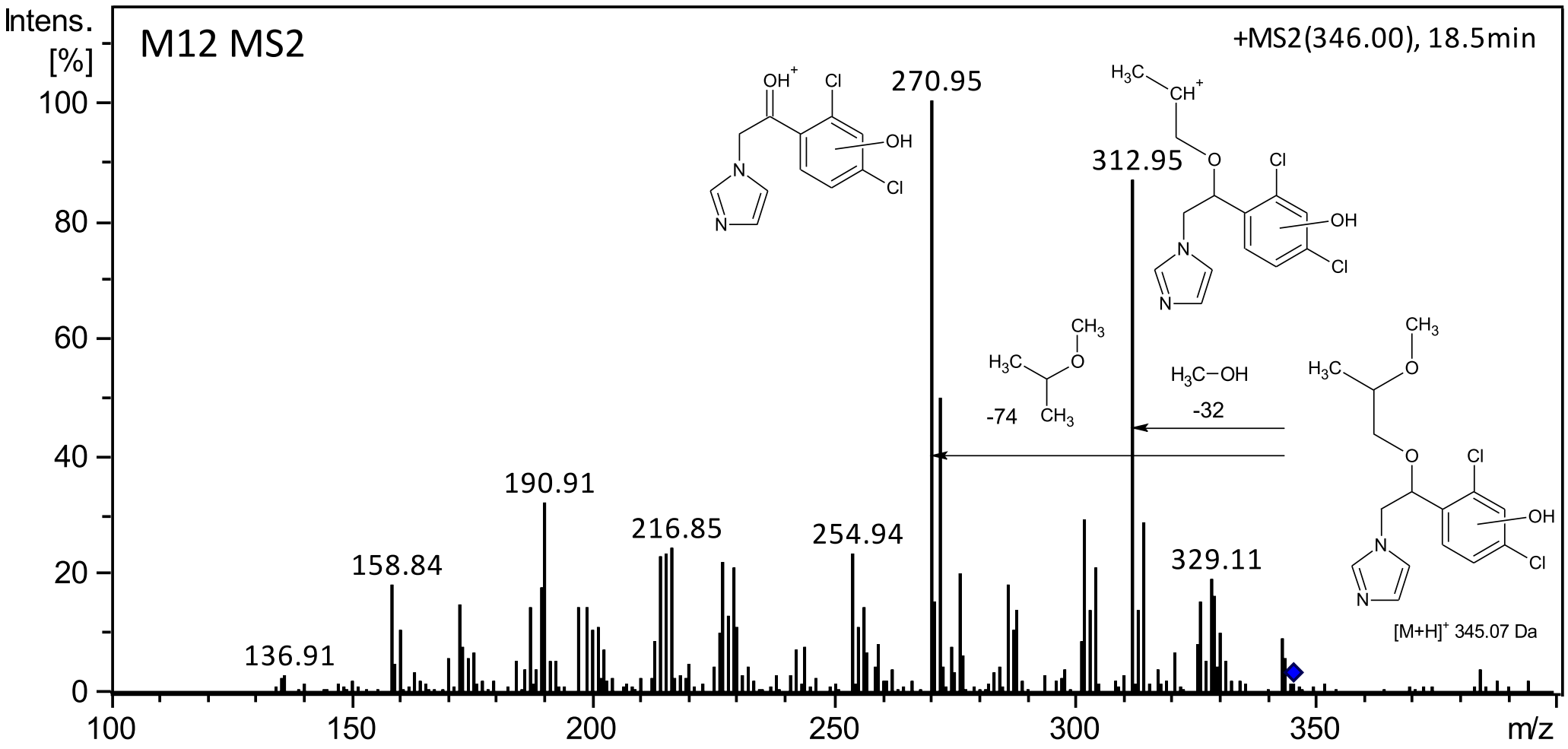

M10 MS3
+MS3(314.00->272.00), 17.0min
Intens.
[%]
100
80
60
40
20
0
174.79
202.79
270.88
143.26
227.90
252.80
289.88
-28 CO
-68
100
150
200
250
300
350
m/z

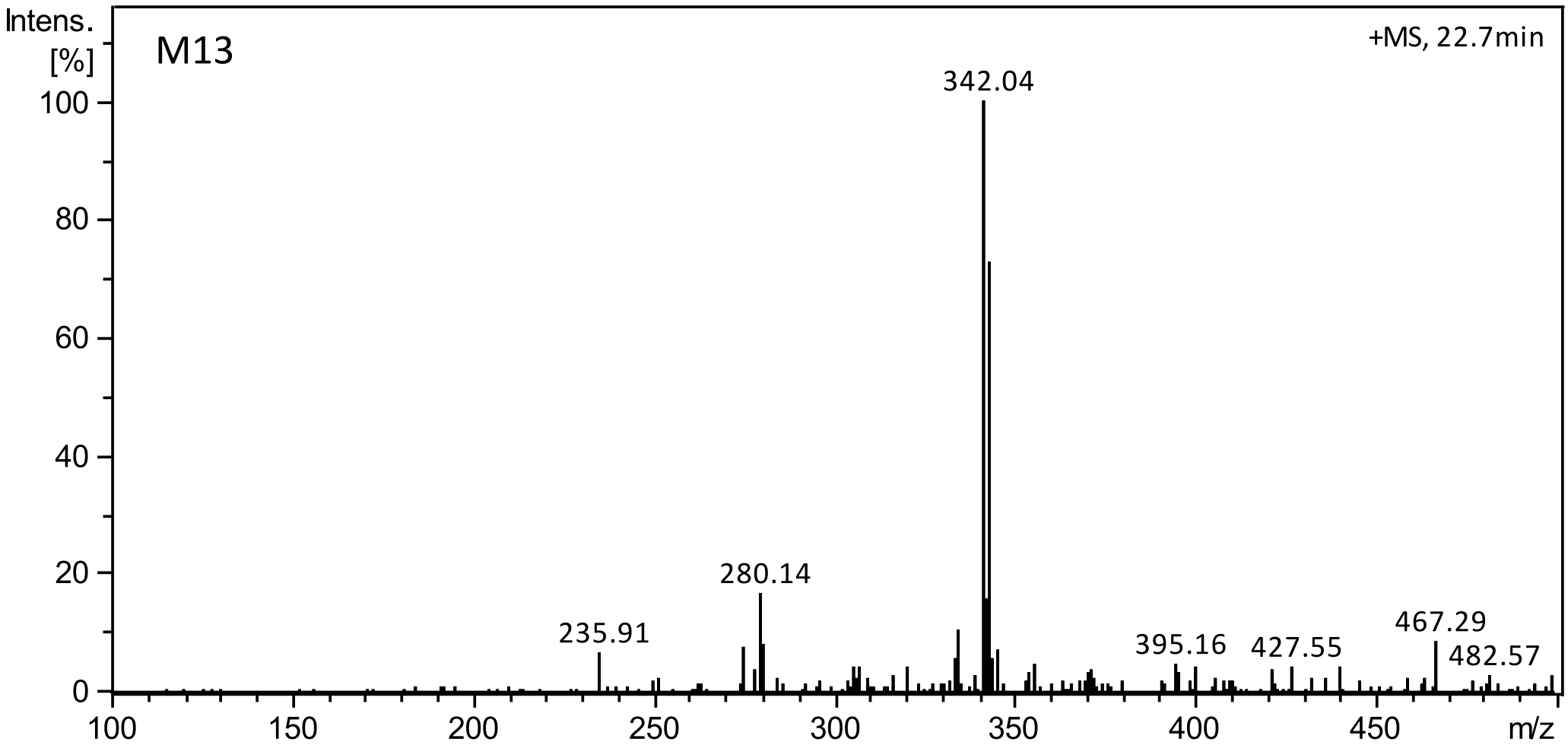

Intens.
[%]
M11
+MS, 17.1min
426.19
313.00
366.18
457.05
268.93
195.94
335.17
150.84
225.52
100
80
60
40
20
0
100
150
200
250
300
350
400
450
m/z

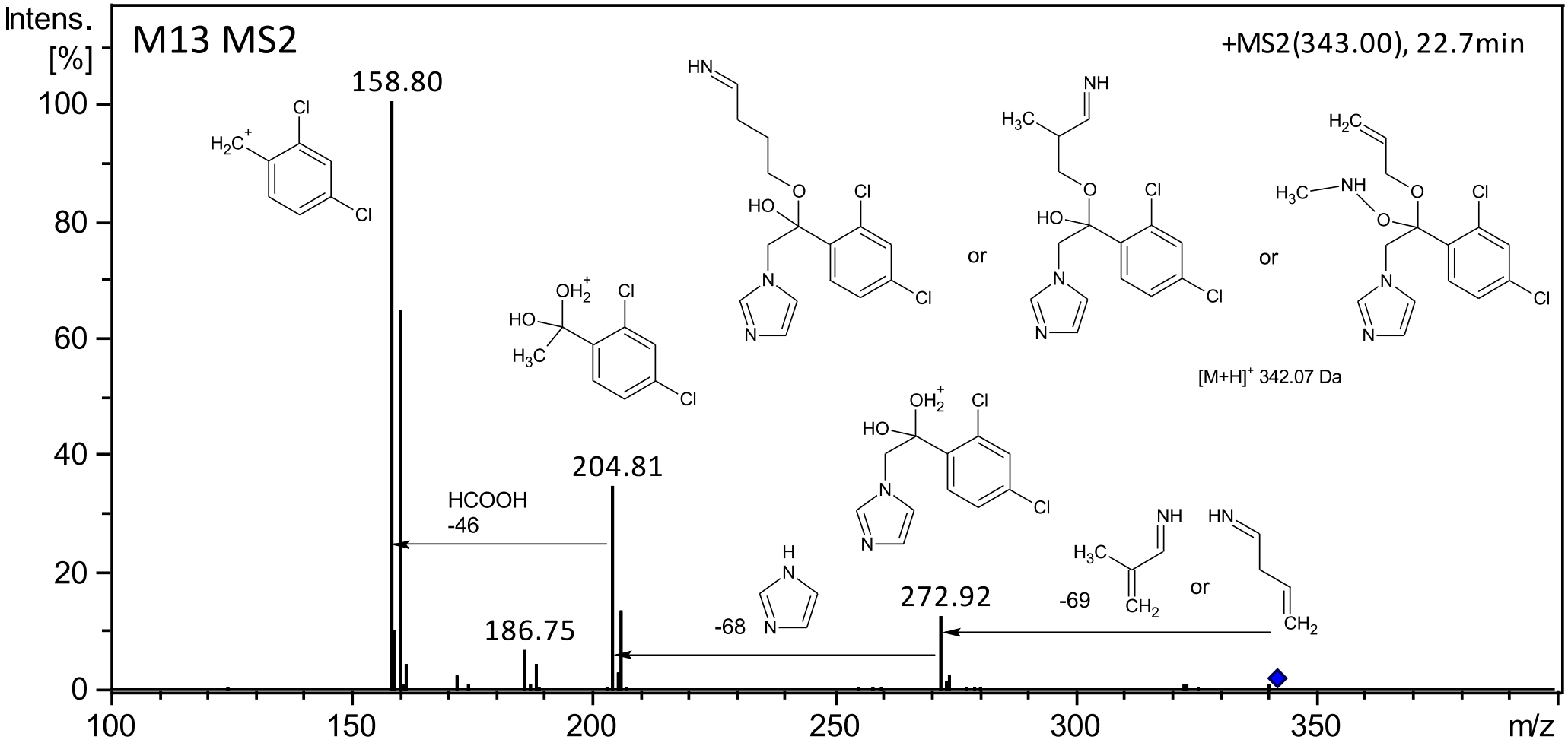

M11 MS2
+MS2(314.00), 17.1min
Intens.
[%]
100
80
60
40
20
0
100
150
200
250
300
350
m/z
270.86
191.82
162.84
243.83
313.13
-42
[M+H]+ 313.05 Da

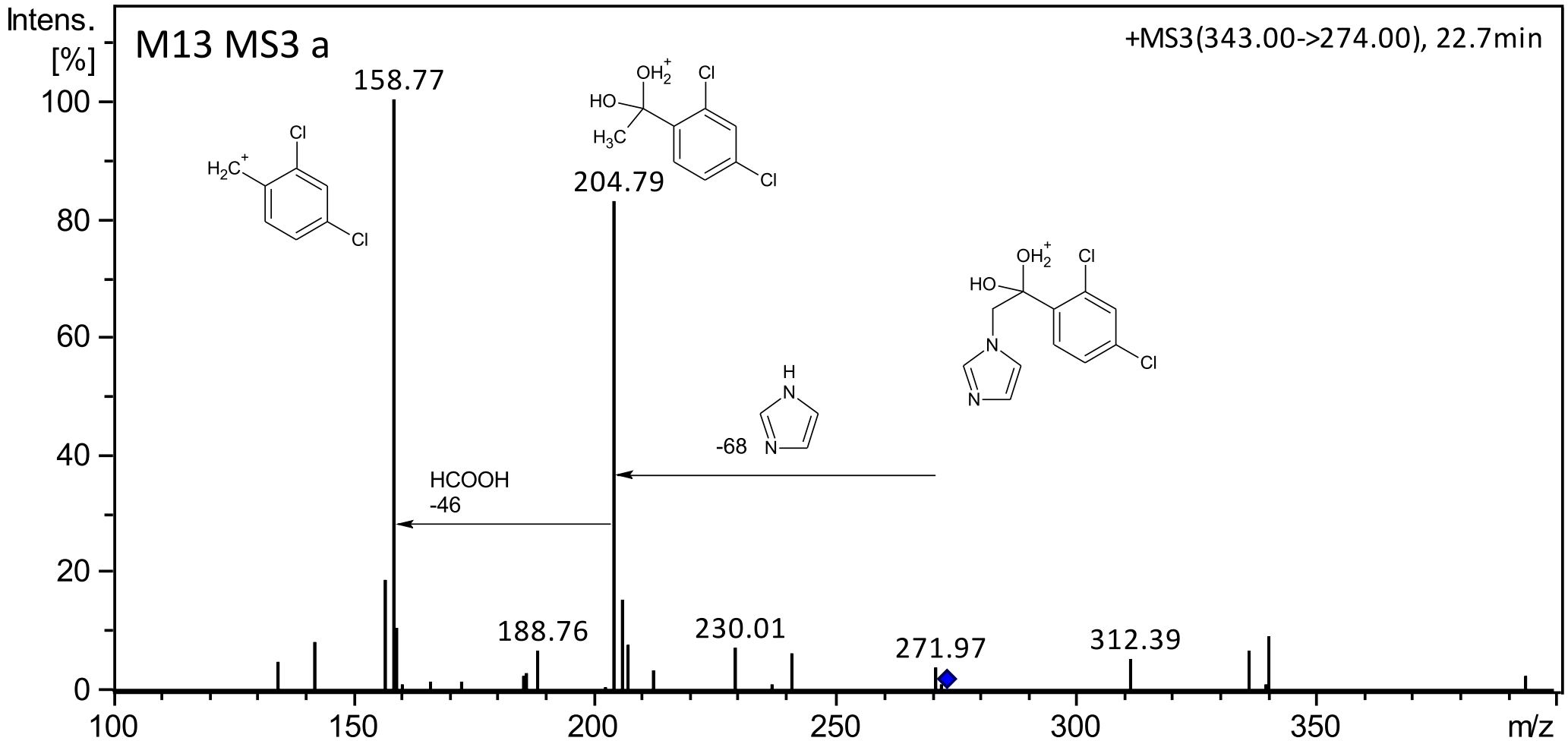

M11 MS3
+MS3(314.00->272.00), 17.1min
Intens.
[%]
100
80
60
40
20
0
100
150
200
250
300
350
m/z
174.79
202.76
270.87
-28 CO
-68
Cl
OH
Cl
H2C+
O
H
N
N

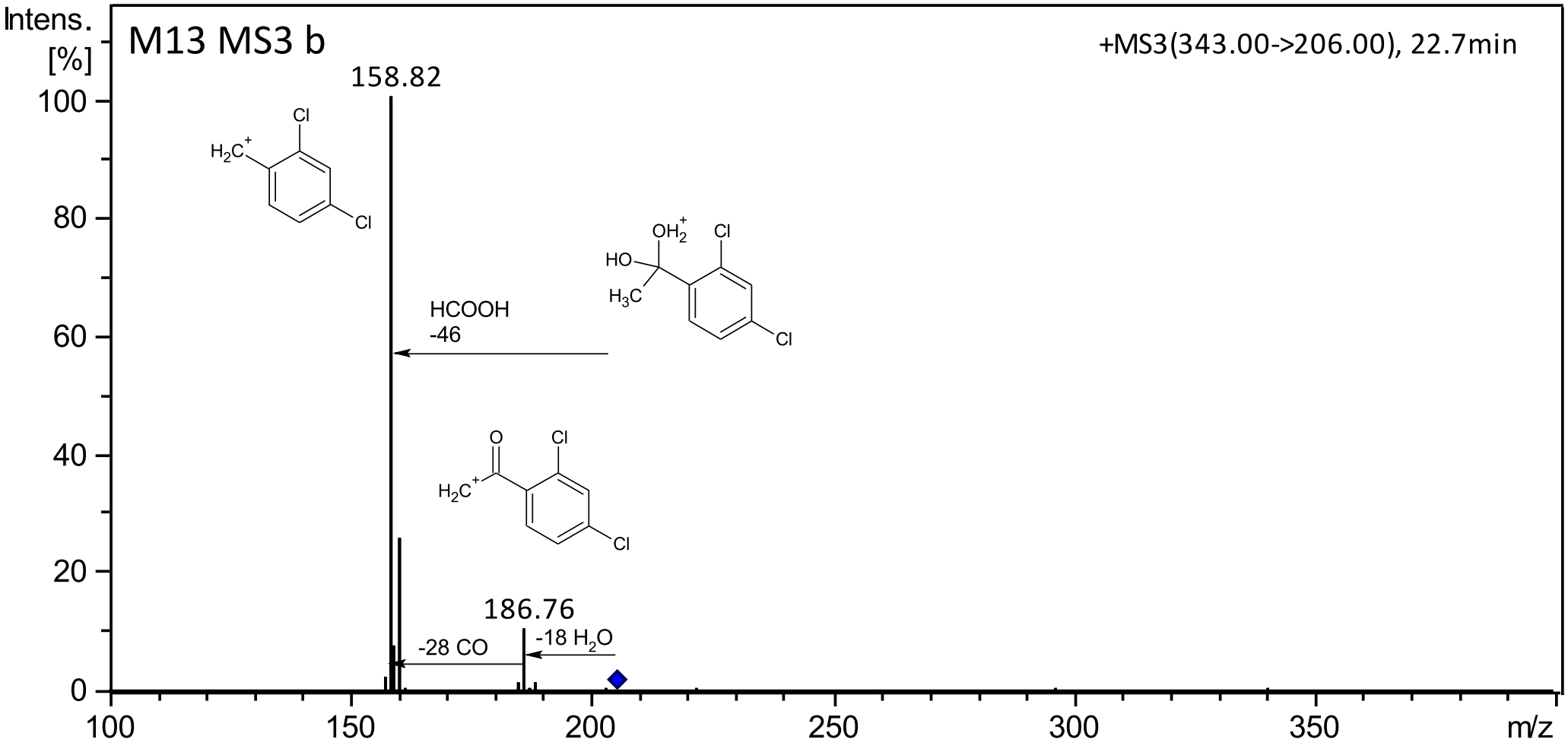

Intens.
[%]
M12
+MS, 18.5min
345.05
238.00
473.95
411.73
146.79
216.88
121.80
164.86
100
80
60
40
20
0
100
150
200
250
300
350
400
450
m/z

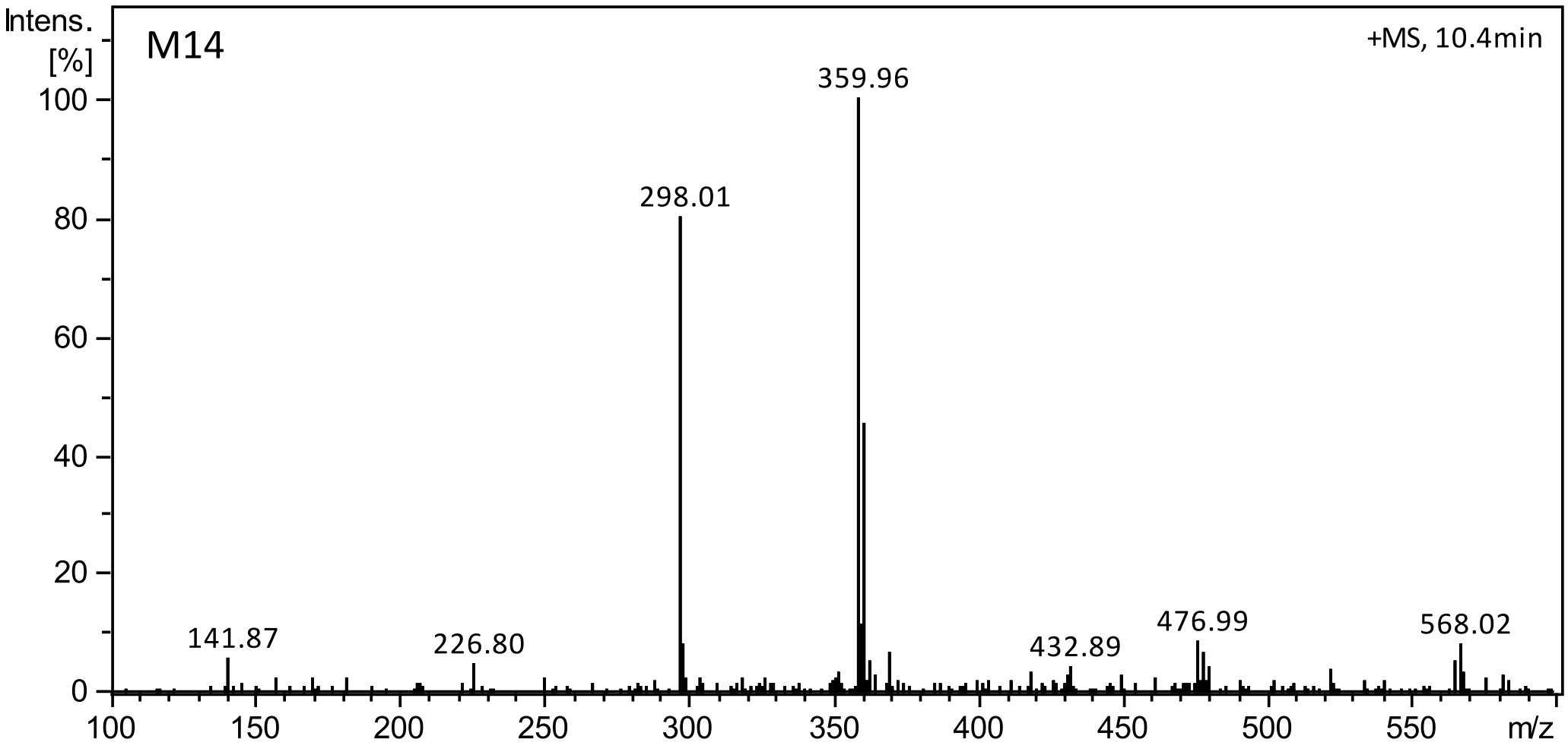

M12 MS2
+MS2(346.00), 18.5min
Intens.
[%]
100
80
60
40
20
0
100
150
200
250
300
350
m/z
136.91
158.84
190.91
216.85
254.94
270.95
312.95
329.11
-74
H3C–OH
-32
[M+H]+ 345.07 Da

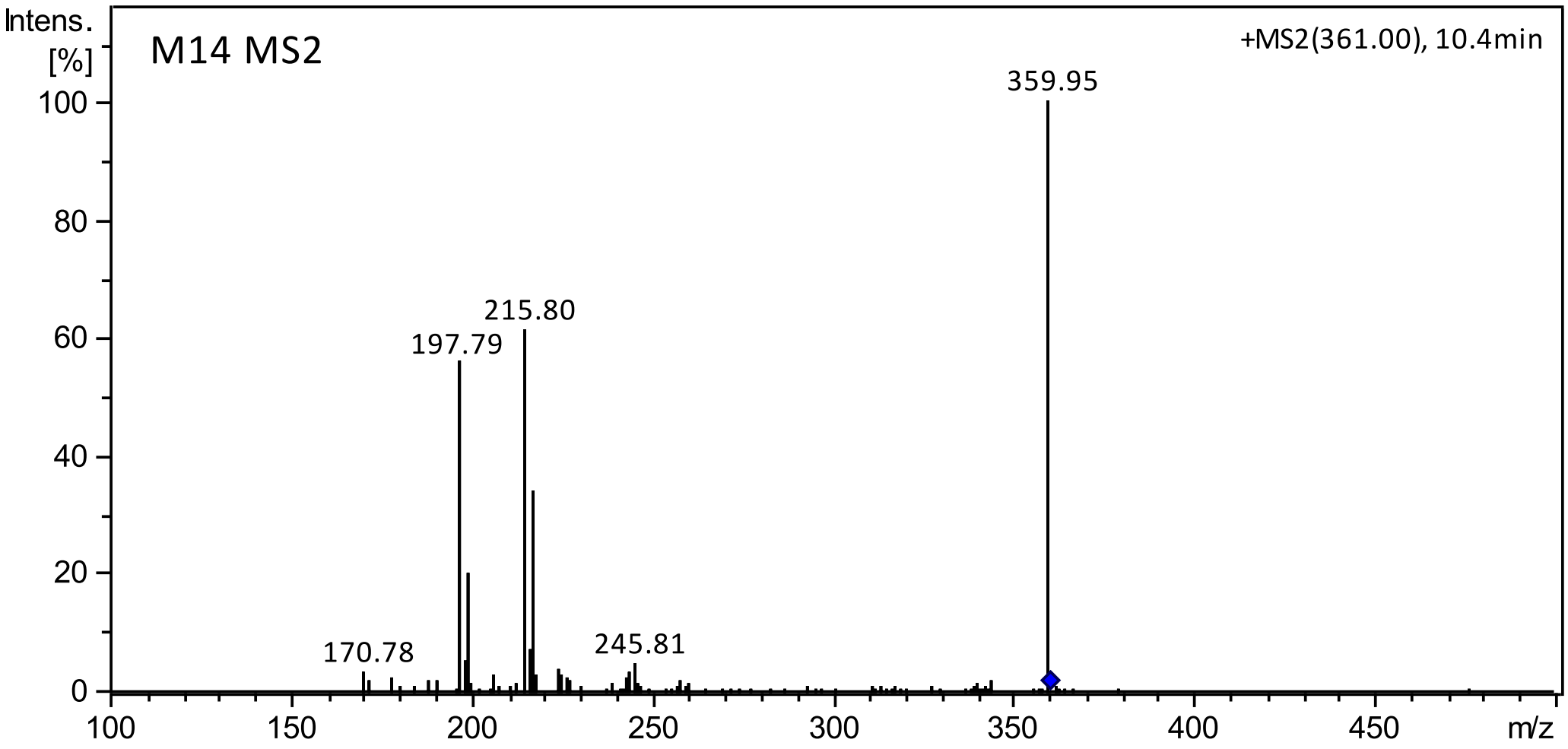

Intens.
[%]
M13
+MS, 22.7min
342.04
280.14
235.91
395.16
427.55
467.29
482.57
100
80
60
40
20
0
100
150
200
250
300
350
400
450
m/z

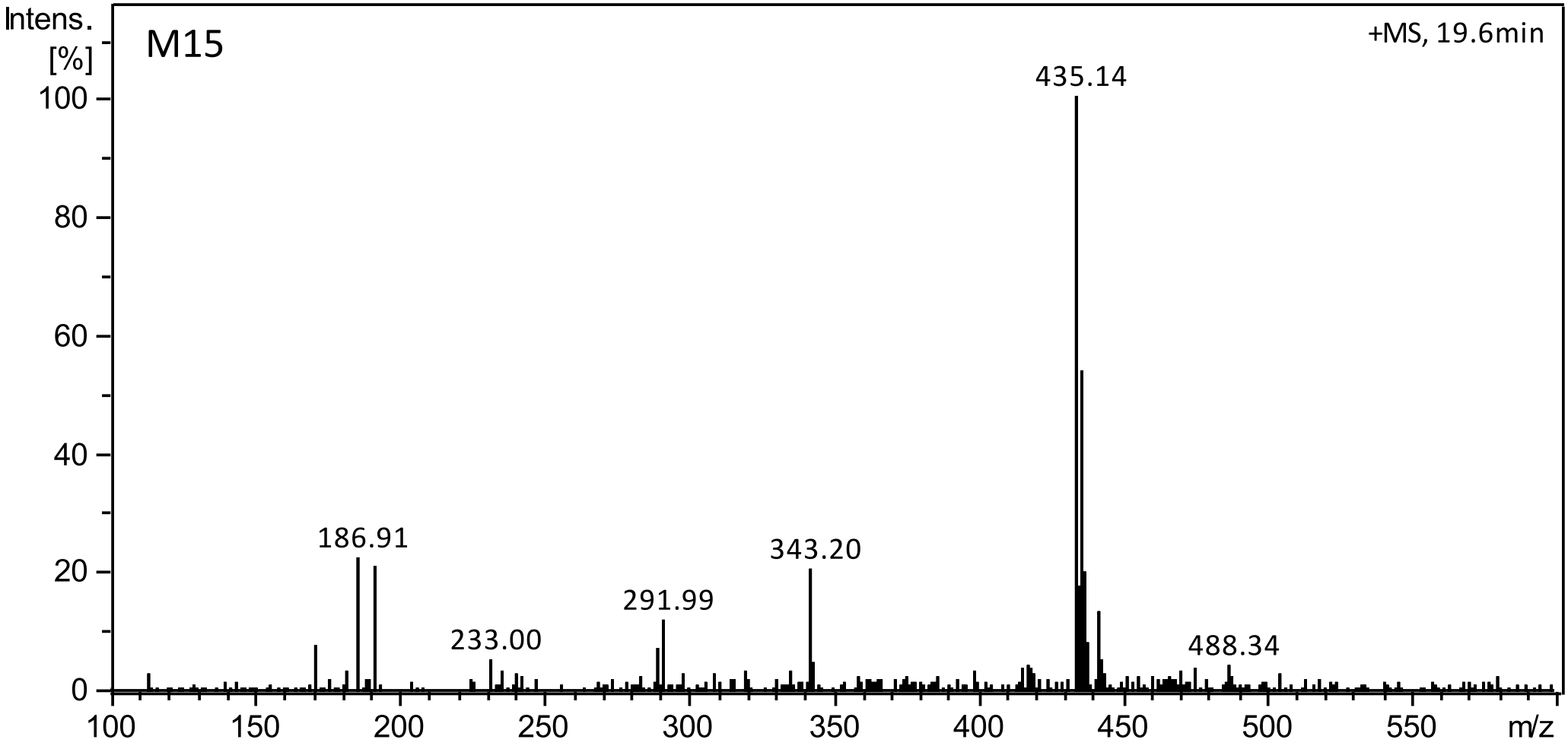

M13 MS2
+MS2(343.00), 22.7min
Intens. [%]
158.80
204.81
186.75
272.92
HCOOH
-46
-68
-69
or
or
[M+H]+ 342.07 Da
m/z

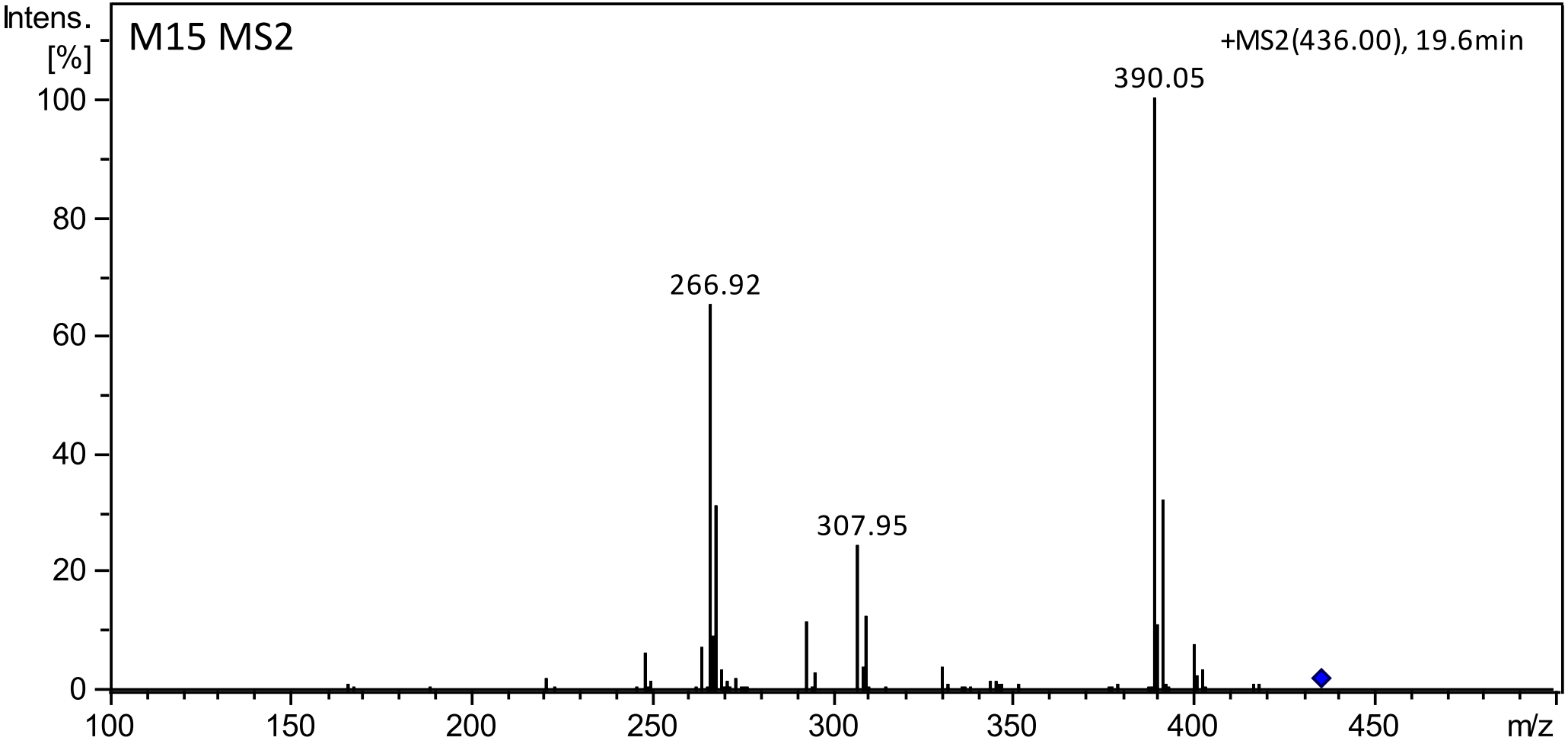

M13 MS3 a
+MS3(343.00->274.00), 22.7min
Intens.
[%]
158.77
204.79
188.76
230.01
271.97
312.39
HCOOH
-46
-68
m/z

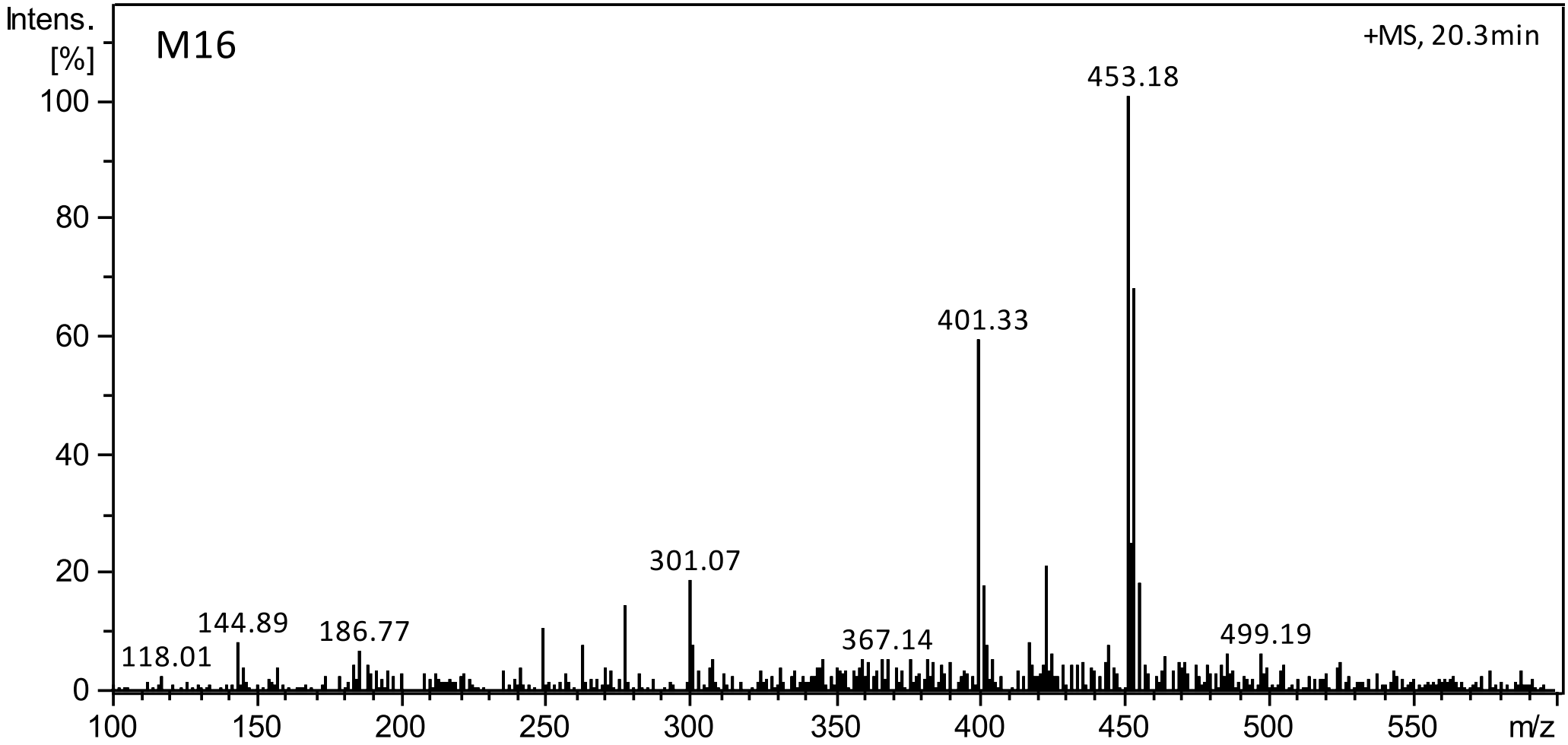

M13 MS3 b
+MS3(343.00->206.00), 22.7min
Intens.
[%]
158.82
186.76
HCOOH
-46
-28 CO
-18 H2O
m/z
100
80
60
40
20
0
100
150
200
250
300
350

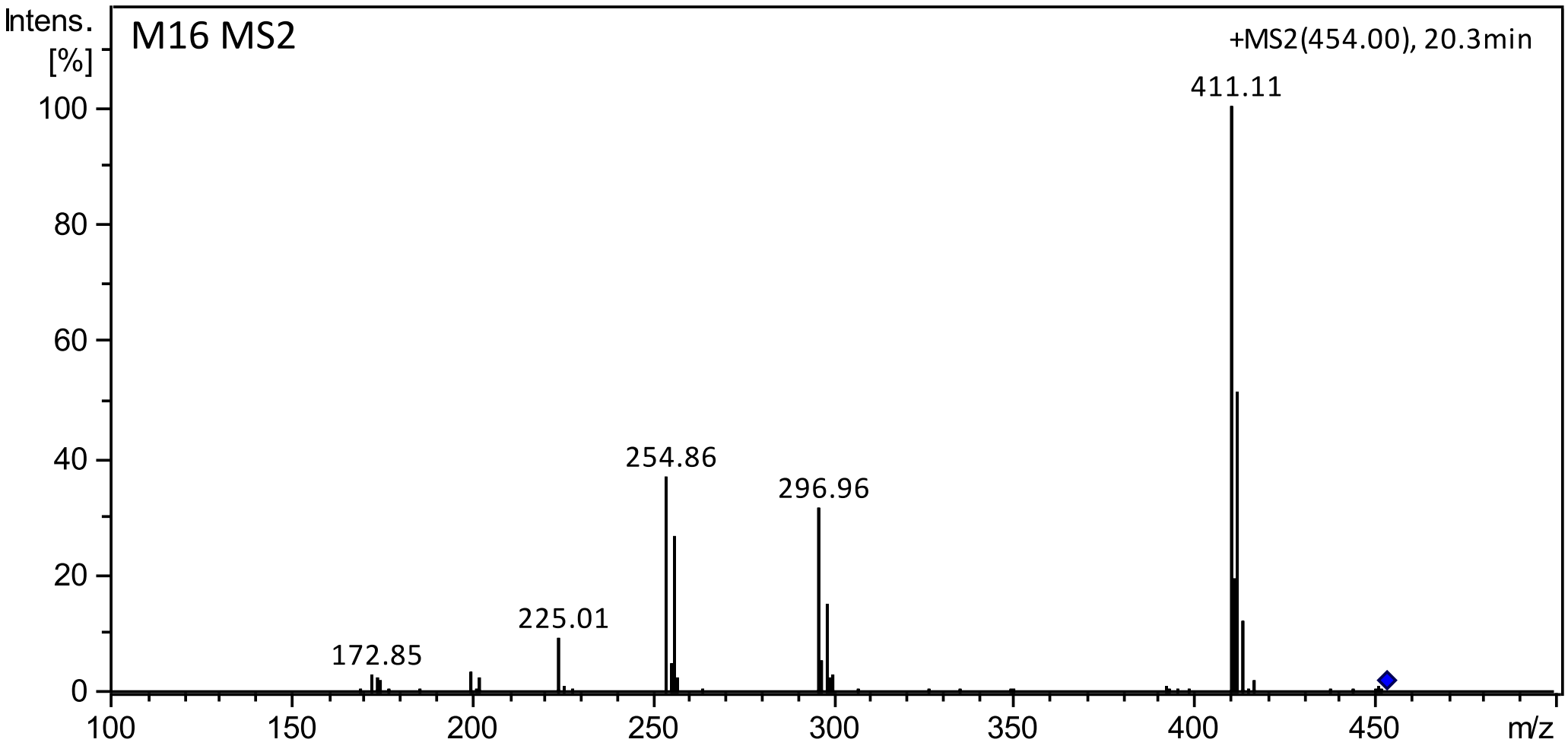

M14
+MS, 10.4min
Intens.
[%]
100
80
60
40
20
0
359.96
298.01
141.87
226.80
432.89
476.99
568.02
100
150
200
250
300
350
400
450
500
550
m/z


M14 MS2
+MS2(361.00), 10.4min
Intens.
[%]
100
80
60
40
20
0
359.95
215.80
197.79
170.78
245.81
100
150
200
250
300
350
400
450
m/z


M15
+MS, 19.6min
Intens.
[%]
100
80
60
40
20
0
435.14
186.91
343.20
291.99
233.00
488.34
100
150
200
250
300
350
400
450
500
550
m/z


M15 MS2
+MS2(436.00), 19.6min
Intens.
[%]
100
80
60
40
20
0
390.05
266.92
307.95
100
150
200
250
300
350
400
450
m/z


M16
+MS, 20.3min
Intens.
[%]
100
80
60
40
20
0
453.18
401.33
301.07
144.89
186.77
118.01
367.14
499.19
100
150
200
250
300
350
400
450
500
550
m/z


M16 MS2
+MS2(454.00), 20.3min
Intens.
[%]
100
80
60
40
20
0
411.11
254.86
296.96
225.01
172.85
100
150
200
250
300
350
400
450
m/z