Electronic Supplementary Material (ESI) for Analytical Methods.


# Supplemental figures

## A practical strategy for chemical profiling of herbal medicines using ultra-high performance liquid chromatography coupled with hybrid triple quadrupole-linear ion trap mass spectrometry: a case study of Mori Cortex

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**Fig. S1** Representative compounds for six types of Diels-Alder type adducts.

**Fig. S2** $MS^2$ spectra, the chemical structures and the fragment ions assignment of morin-*di*-*O*-glucoside.

**Fig. S3** $MS^2$ spectra, the chemical structures and the fragment ions assignment of morin-*di*-*O*-glucoside oxyresveratrol-*O*-glucoside.

**Fig. S4** $MS^2$ spectra, the chemical structures and the fragment ions assignment of moracin M (A), moracin M-*O*-glucoside (B) and moracin M-*di*-*O*-glucoside (C).

**Fig. S5** $MS^2$ spectra , the chemical structures and the fragment ions assignment of moracin O (A), moracin O-*O*-glucoside (B) and moracin O-*O*-xyloside (C).

**Fig. S6** $MS^2$ spectra, the chemical structures and the fragment ions assignment of moracin P (A), and moracin P-*O*-glucoside (B).

**Fig. S7** $MS^2$ spectrum of albafuran C (A) and the proposed mass fragmentation scheme under negative ionization (B).

**Fig. S8** $MS^2$ spectrum of kuwanon C (A) and the proposed mass fragmentation scheme under positive ionization (B).

**Fig. S9** $MS^2$ spectrum of sanggenol B (A) and the proposed mass fragmentation scheme under positive ionization (B).

Kuwanon L

Mulberrofuran C

Kuwanon P

Kuwanon Q

Guangsangon L

Dimoracin

Fig. S1

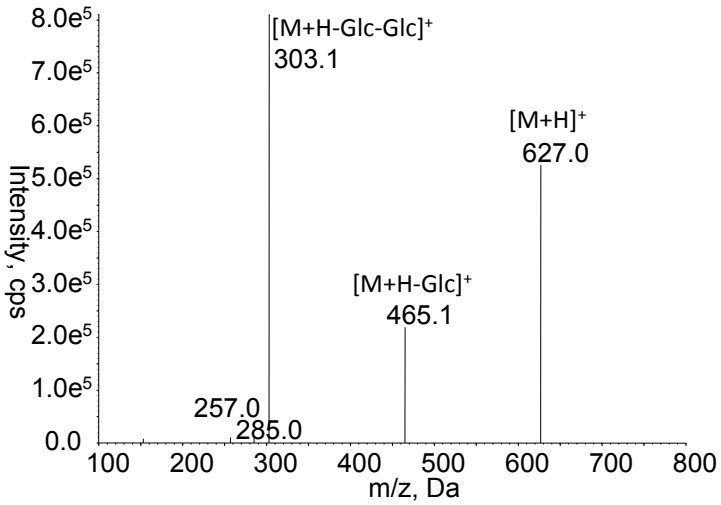

8.0e5
7.0e5
6.0e5
5.0e5
4.0e5
3.0e5
2.0e5
1.0e5
0.0
Intensity, cps
[M+H-Glc-Glc]+
303.1
[M+H]+
627.0
[M+H-Glc]+
465.1
257.0
285.0
100
200
300
400
500
600
700
800
m/z, Da

Fig. S2

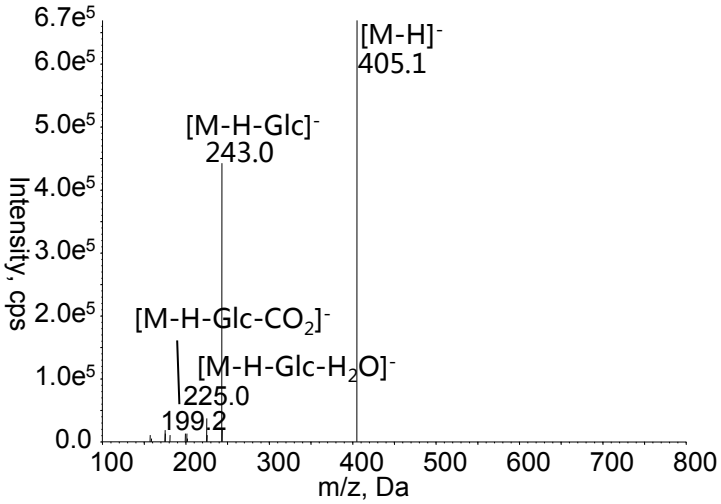
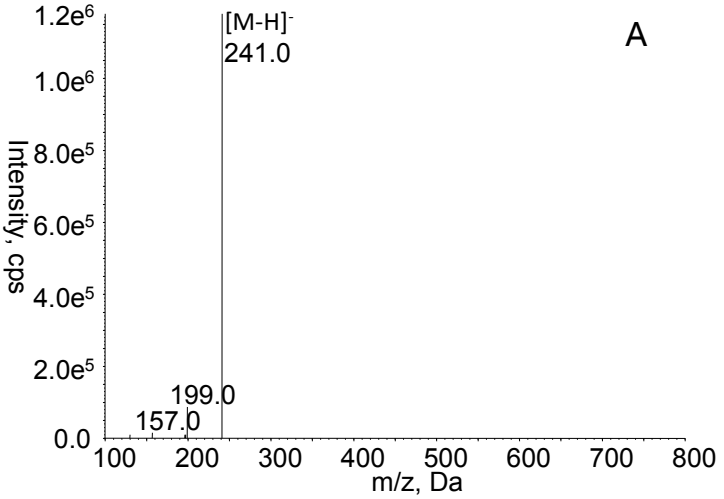
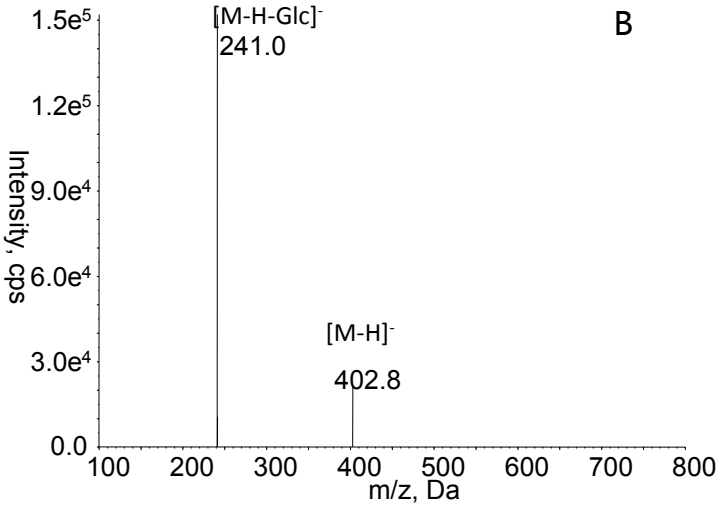

6.7e5
6.0e5
5.0e5
4.0e5
3.0e5
2.0e5
1.0e5
0.0
Intensity, cps
[M-H]-
405.1
[M-H-Glc]-
243.0
[M-H-Glc-CO2]-
225.0
[M-H-Glc-H2O]-
199.2
100
200
300
400
500
600
700
800
m/z, Da

Fig. S3


A
[M-H]-
241.0
199.0
157.0
Intensity, cps
m/z, Da


B
[M-H-Glc]-
241.0
[M-H]-
402.8
Intensity, cps
m/z, Da

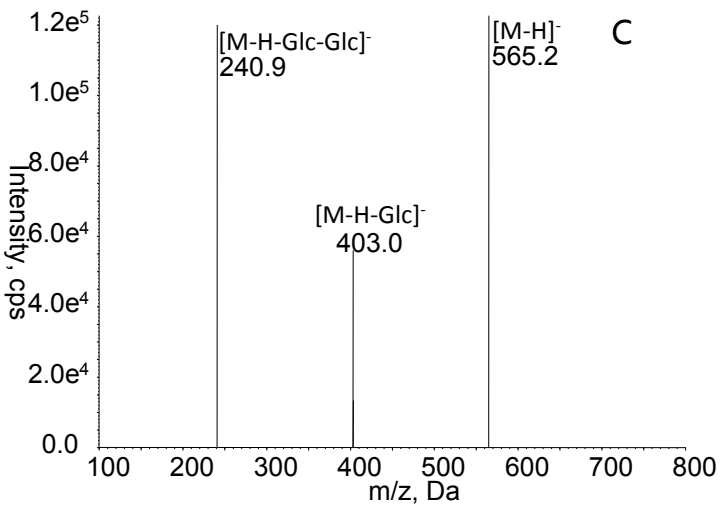

C
[M-H-Glc-Glc]-
240.9
[M-H]-
565.2
[M-H-Glc]-
403.0
Intensity, cps
m/z, Da

Fig. S4

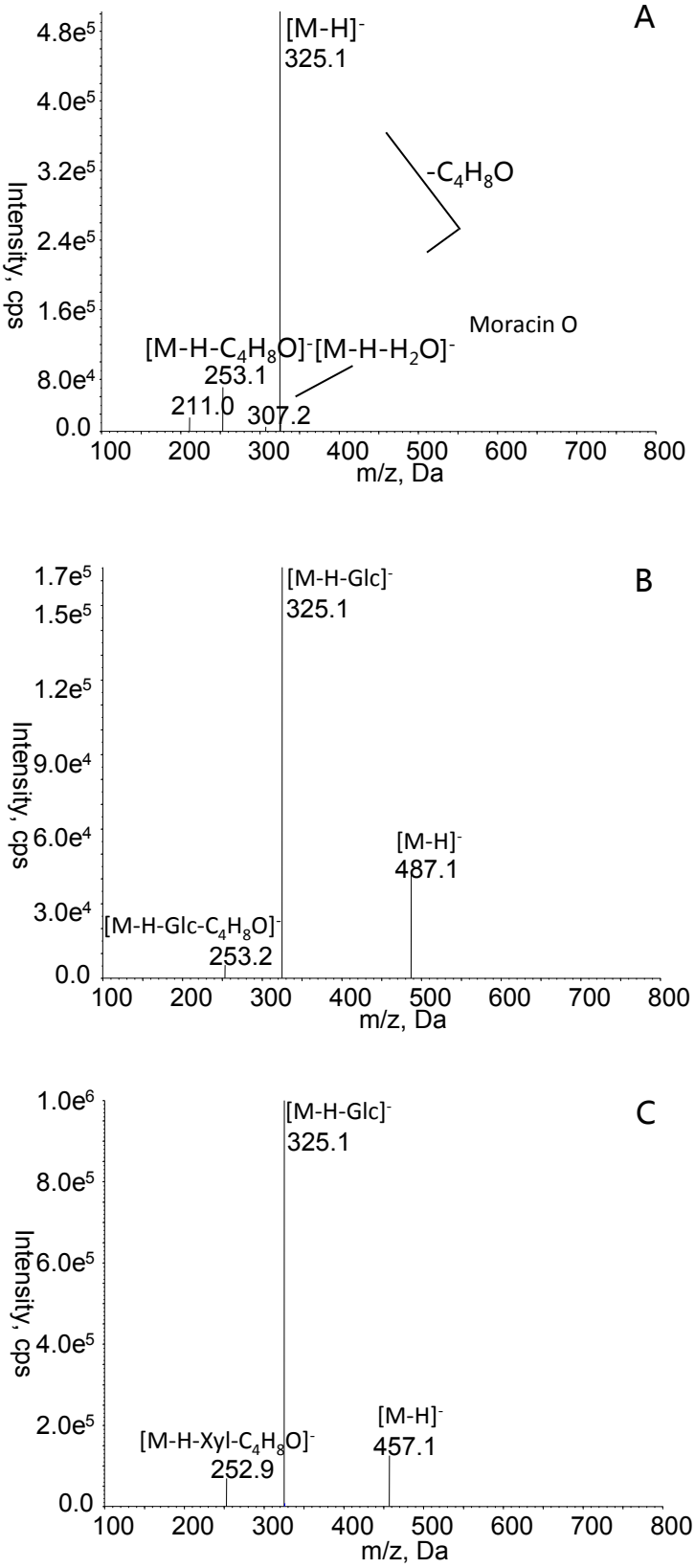
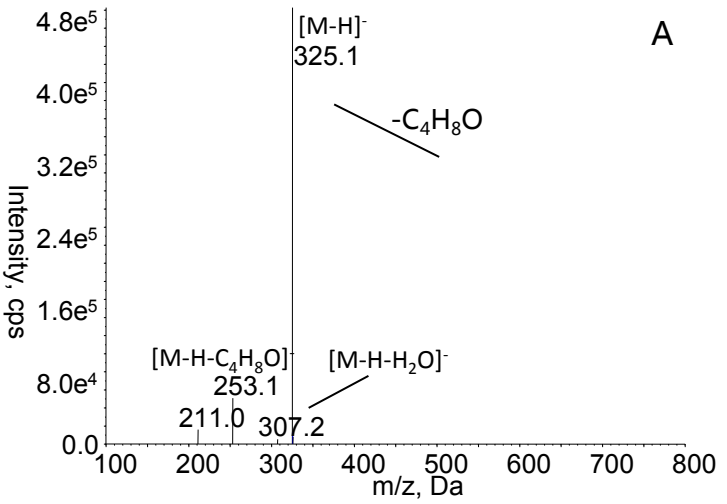

A
[M-H]-
325.1
-C4H8O
Moracin O
[M-H-C4H8O]-
253.1
211.0
[M-H-H2O]-
307.2
Intensity, cps
m/z, Da
B
[M-H-Glc]-
325.1
[M-H]-
487.1
[M-H-Glc-C4H8O]-
253.2
Intensity, cps
m/z, Da
C
[M-H-Glc]-
325.1
[M-H]-
457.1
[M-H-Xyl-C4H8O]-
252.9
Intensity, cps
m/z, Da

Fig. S5


A
[M-H]-
325.1
-C4H8O
[M-H-C4H8O]-
253.1
211.0
307.2
[M-H-H2O]-
Intensity, cps
m/z, Da

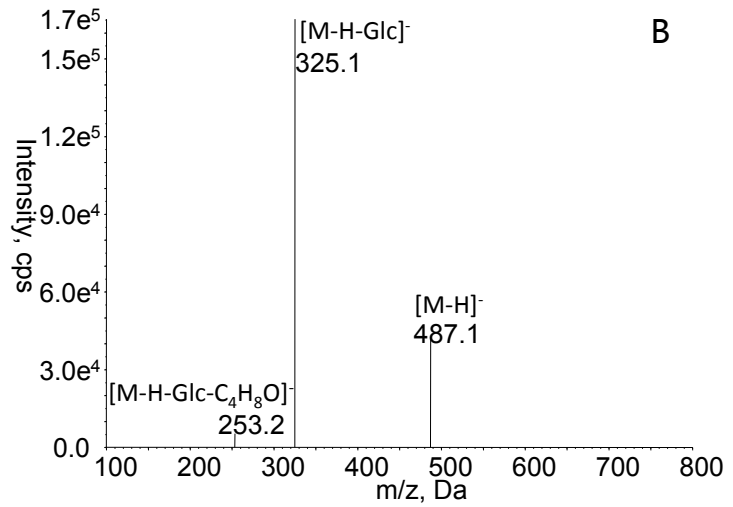
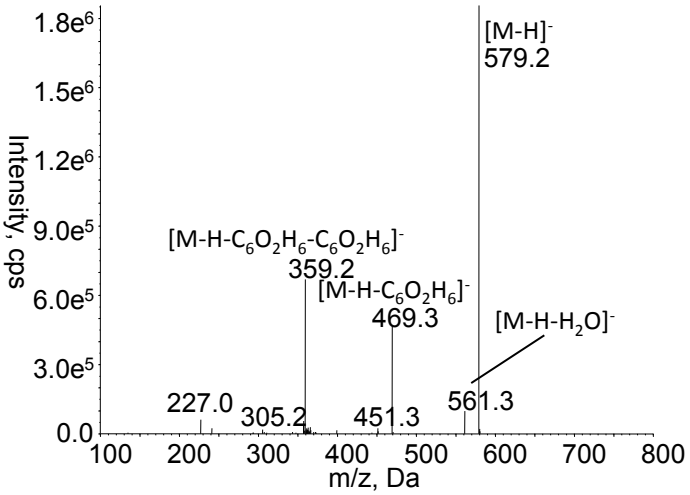

B
[M-H-Glc]-
325.1
[M-H]-
487.1
[M-H-Glc-C4H8O]-
253.2
Intensity, cps
m/z, Da

Fig. S6

A


1.8e6
1.5e6
1.2e6
9.0e5
6.0e5
3.0e5
0.0
Intensity, cps
[M-H]-
579.2
[M-H-C6O2H6-C6O2H6]-
359.2
[M-H-C6O2H6]-
469.3
[M-H-H2O]-
561.3
227.0
305.2
451.3
100
200
300
400
500
600
700
800
m/z, Da

B

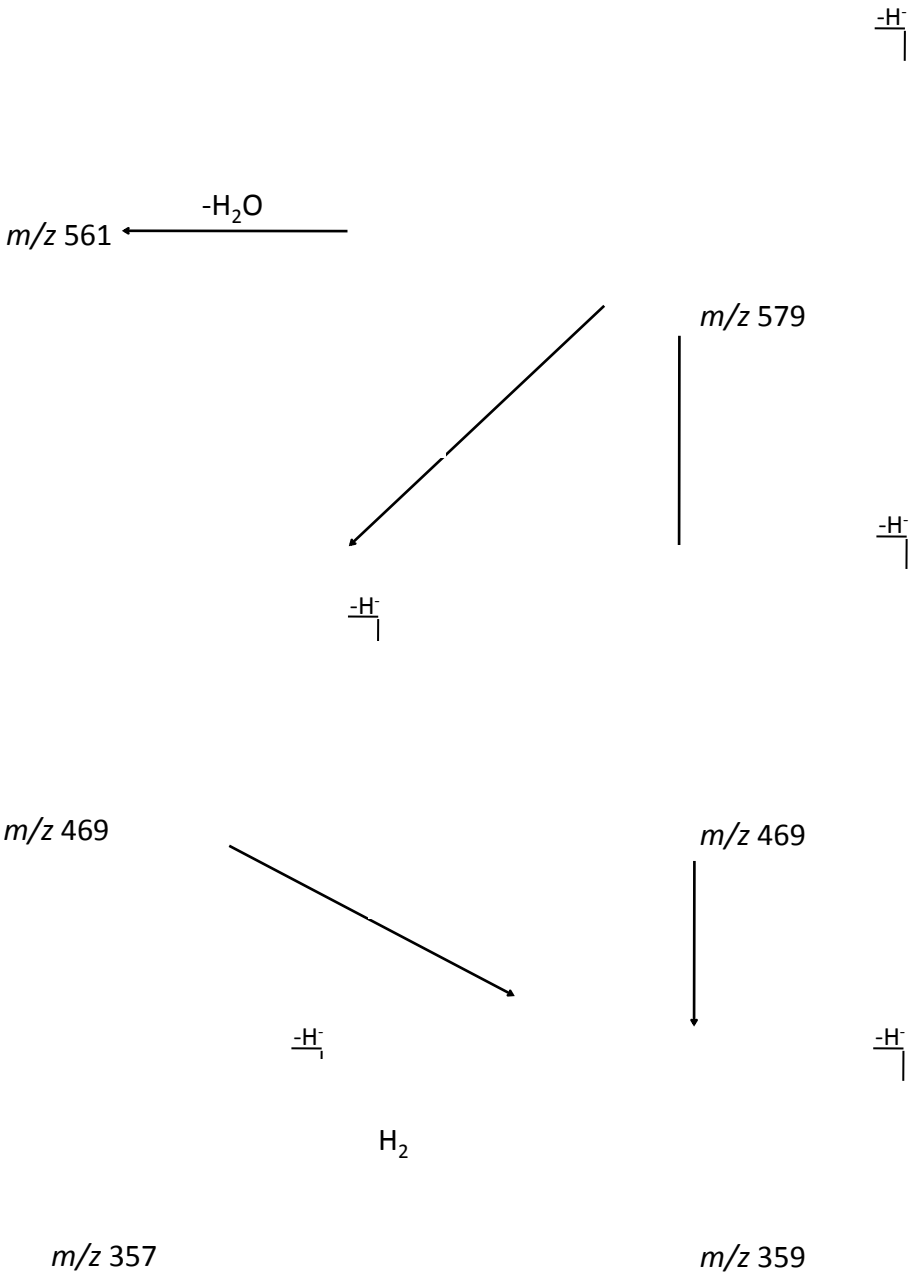

-H2O
m/z 561
m/z 579
-H·
-H·
-H·
m/z 469
m/z 469
-H·
-H·
H2
m/z 357
m/z 359

Fig. S7

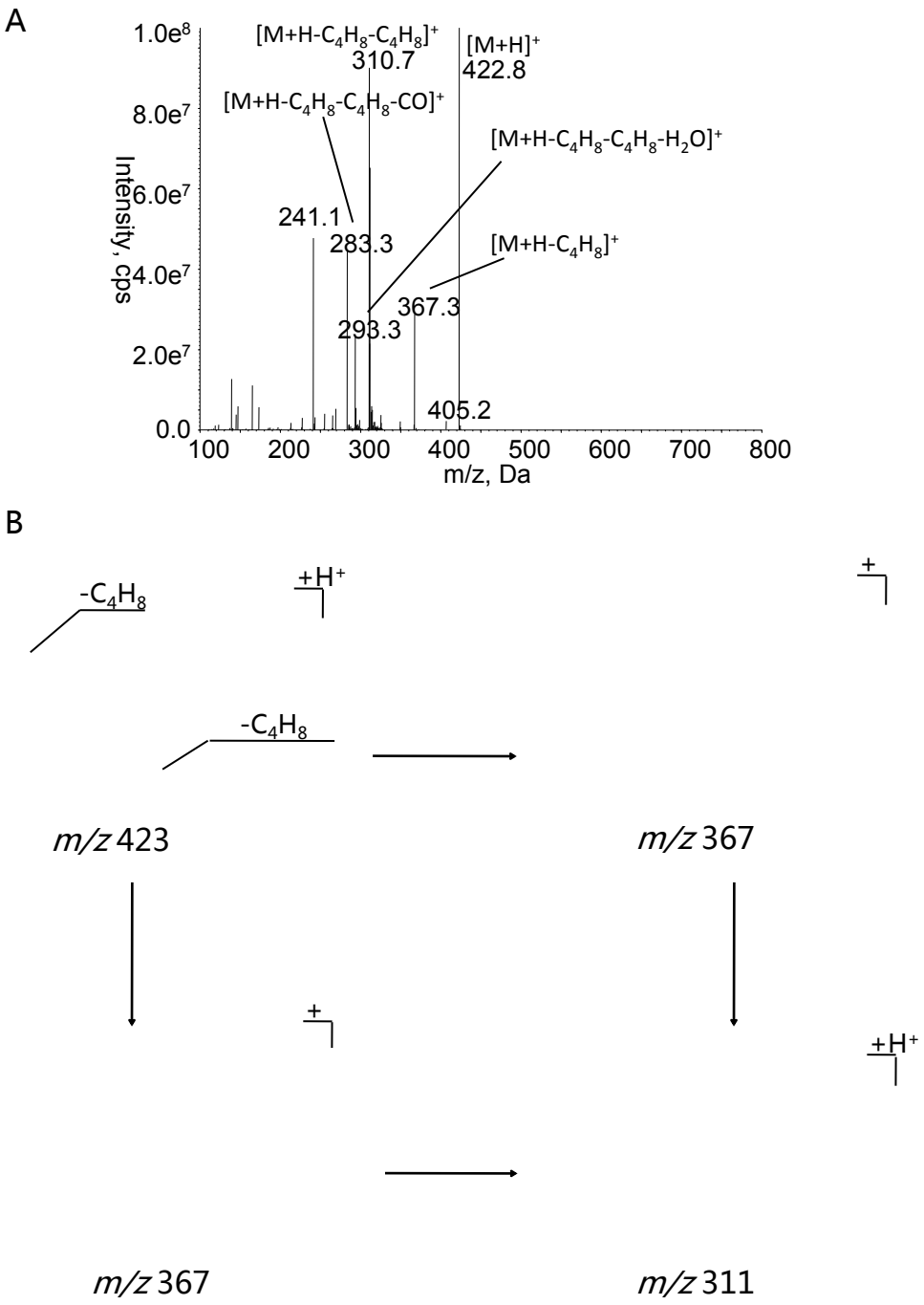
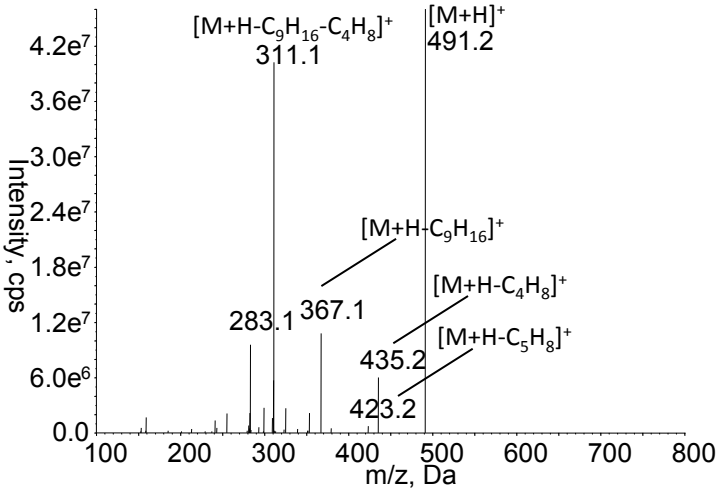

A
1.0e8
8.0e7
6.0e7
4.0e7
2.0e7
0.0
Intensity, cps
[M+H-C4H8-C4H8]+
310.7
[M+H]+
422.8
[M+H-C4H8-C4H8-CO]+
[M+H-C4H8-C4H8-H2O]+
241.1
283.3
[M+H-C4H8]+
367.3
293.3
405.2
100
200
300
400
500
600
700
800
m/z, Da
B
-C4H8
+H+
+
-C4H8
m/z 423
m/z 367
+
+H+
m/z 367
m/z 311

Fig. S8

A


[M+H-C9H16-C4H8]+
311.1
[M+H]+
491.2
[M+H-C9H16]+
367.1
[M+H-C4H8]+
435.2
[M+H-C5H8]+
423.2
283.1
Intensity, cps
4.2e7
3.6e7
3.0e7
2.4e7
1.8e7
1.2e7
6.0e6
0.0
100
200
300
400
500
600
700
800
m/z, Da

B

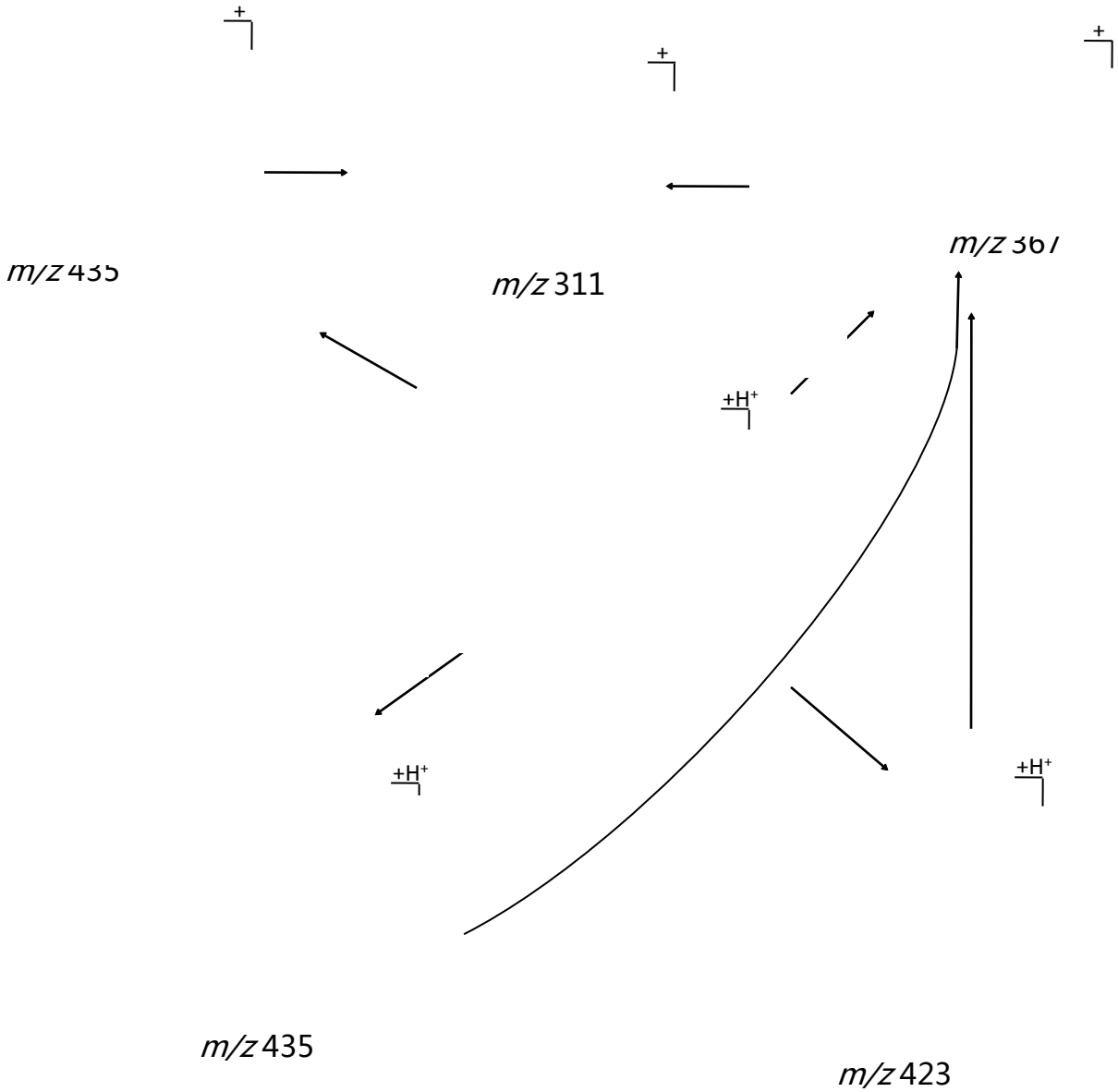

m/z 435
m/z 311
m/z 367
+H+
+H+
+H+
m/z 435
m/z 423

Fig. S9