Electronic Supplementary Material (ESI) for Analytical Methods.

Supplemental information

Direct stability characterization of aconite alkaloids in different mediums by autosampler-mediated incubation–online solid phase extraction–LC–MS/MS

Na Zhang [1,2,3,#], Jun Li [1,#], Shepo Shi [1], Qingqing Song [1,2], Chun Li [1], Yunfang Zhao[1], Yuelin Song [1*], Pengfei Tu [1*]

[1]. *Modern Research Center for Traditional Chinese Medicine, Beijing University of Chinese Medicine, Beijing 100029, China*

[2]. *School of Chinese Materia Medica, Beijing University of Chinese Medicine, Beijing 100102, China*

[3]. *Baotou Medical College, Baotou 014060, China*

[#] These two authors contribute equally to this article.

* Corresponding authors:

Prof. Pengfei Tu

Modern Research Center for Traditional Chinese Medicine, Beijing University of Chinese Medicine, Beijing 100029, China;

Tel./fax: +86-10-8280 2750; *E-mail*: pengfeitu@163.com.

Dr. Yuelin Song

Modern Research Center for Traditional Chinese Medicine, Beijing University of Chinese Medicine, Beijing 100029, China;

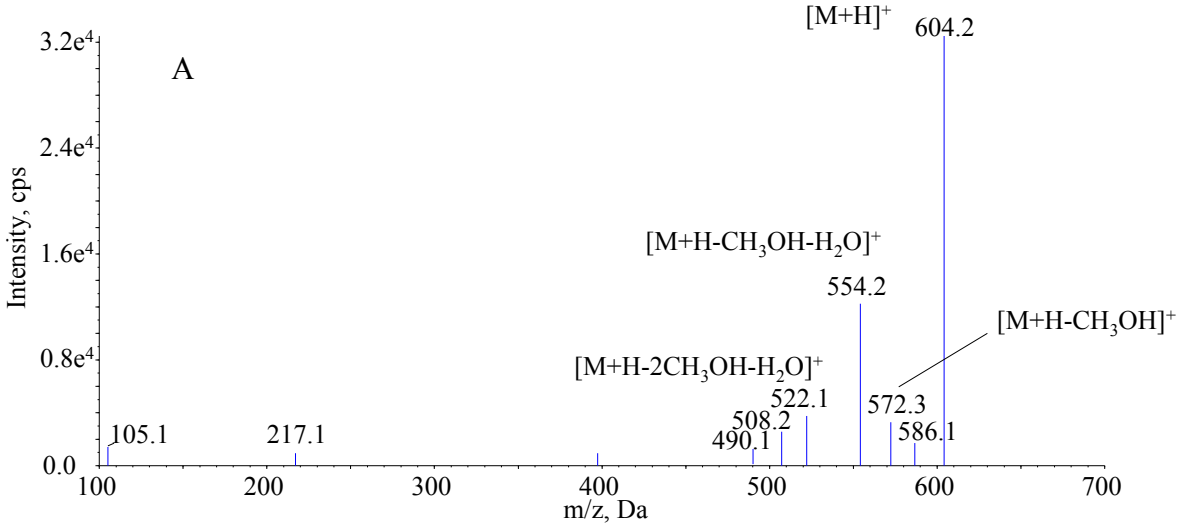
Tel./fax: +86-10-6428 6100; *E-mail*: syltwc2005@163.com.

Figure legends

Fig. S1 A, MS^2 spectrum and assignments of dominant fragments of BAC (benzoylaconitine); B, proposed mass fragmentation pathways of BAC with positive polarity ionization.

Fig. S2 MS^2 spectra and assignments of dominant fragments of mesaconitine (MA) and its two degradation products, namely BMA (benzoylmesaconitine) and pyrmesaconitine. The chemical structures of BMA and pyrmesaconitine are also shown.

Fig. S3 MS^2 spectra and assignments of dominant fragments of hypaconitine (HA) and its two degradation products, namely BHA (benzoylhypaconitine) and pyrhypaconitine. The chemical structures of BHA and pyrhypaconitine are also shown.


A
[M+H]+
604.2
[M+H-CH3OH-H2O]+
554.2
[M+H-CH3OH]+
[M+H-2CH3OH-H2O]+
522.1
572.3
508.2
586.1
490.1
105.1
217.1
Intensity, cps
m/z, Da
3.2e4
2.4e4
1.6e4
0.8e4
0.0
100
200
300
400
500
600
700

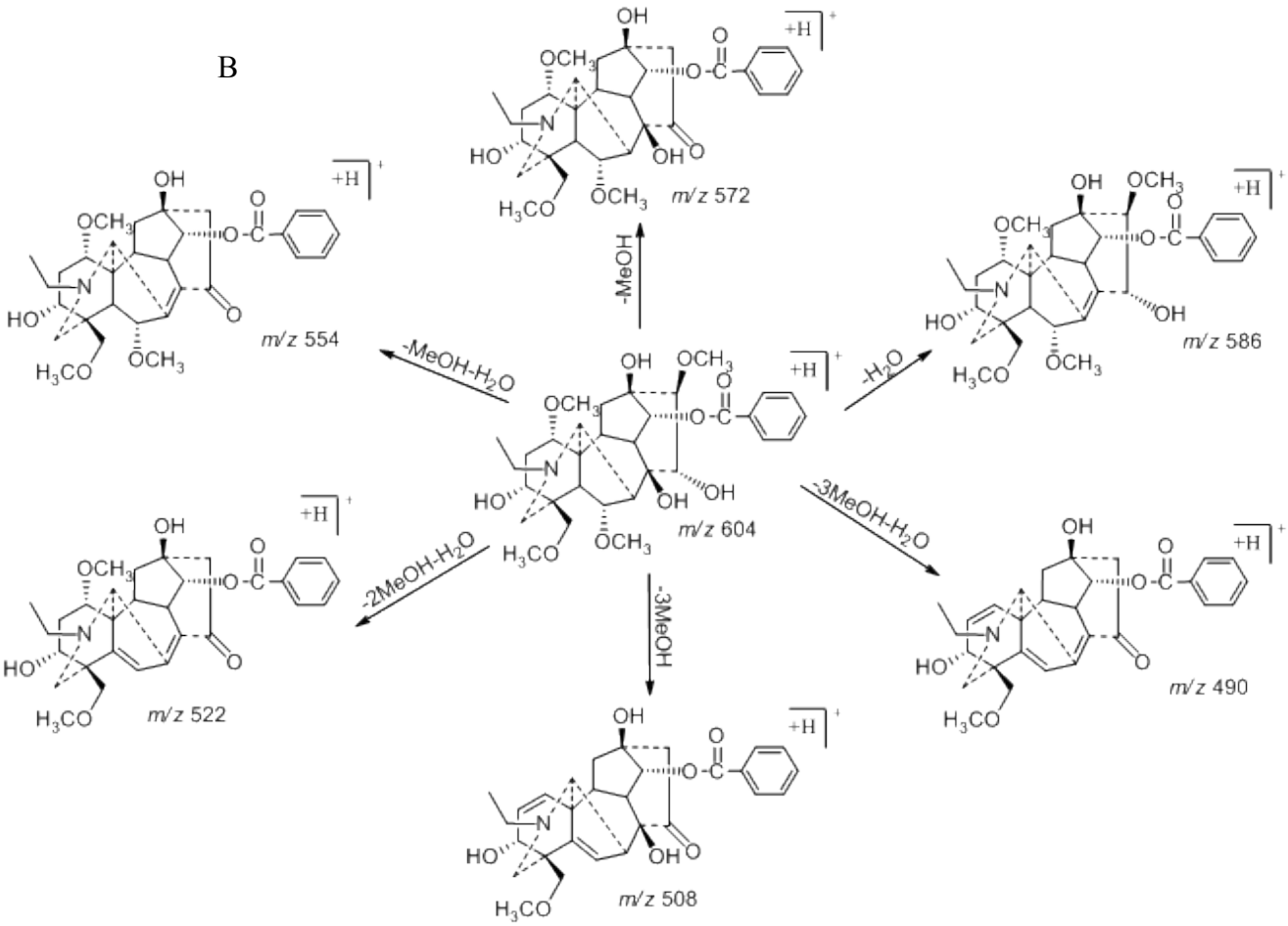
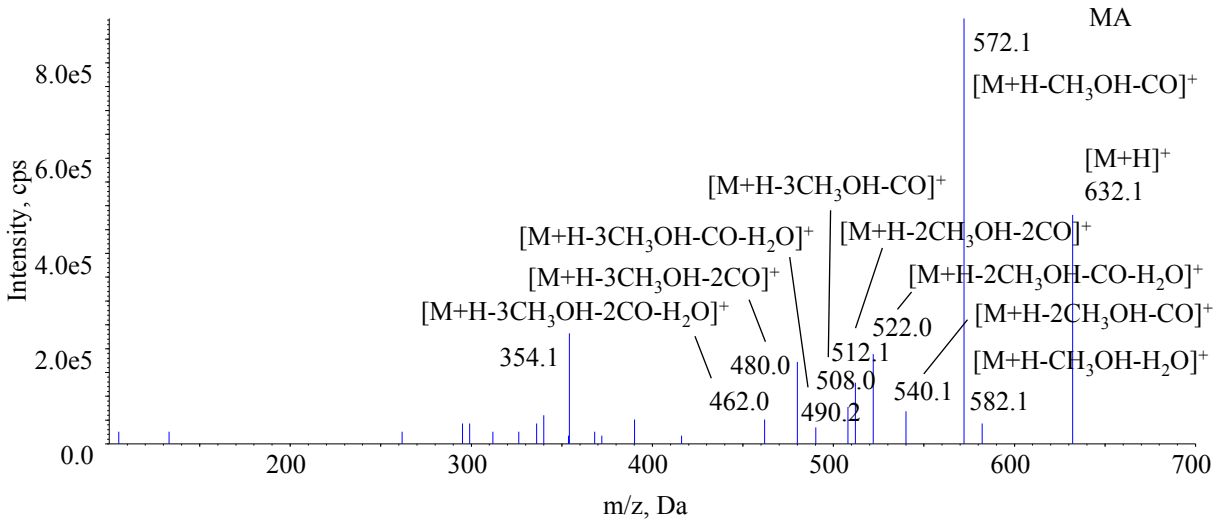
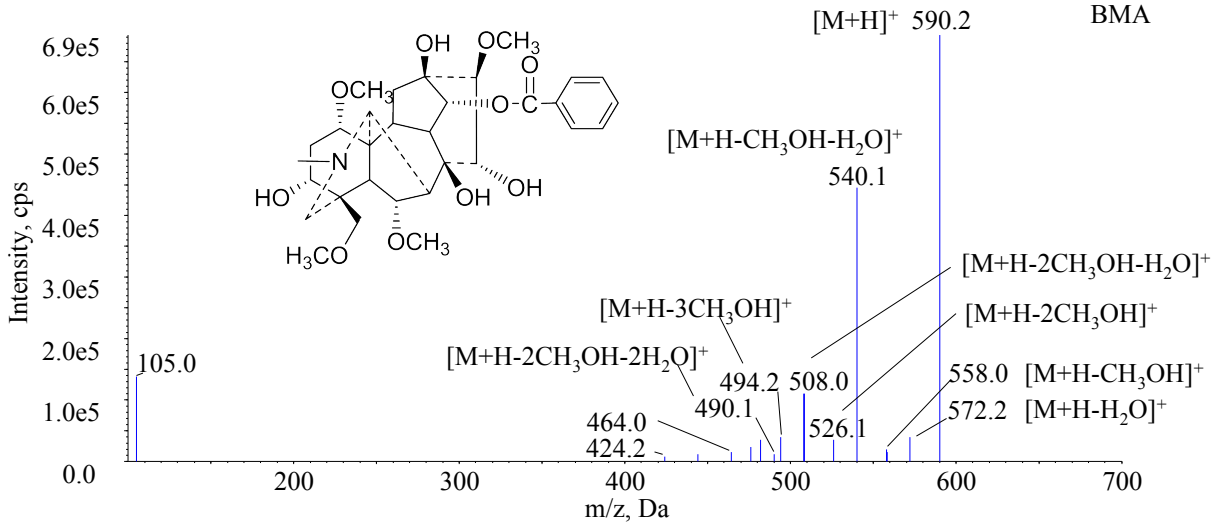

B
m/z 572
m/z 554
m/z 586
m/z 604
m/z 522
m/z 490
m/z 508
-MeOH
-MeOH-H2O
-H2O
-2MeOH-H2O
-3MeOH-H2O
-3MeOH

Fig. S1


MA
572.1
[M+H-CH3OH-CO]+
[M+H]+
632.1
[M+H-3CH3OH-CO]+
[M+H-3CH3OH-CO-H2O]+
[M+H-2CH3OH-2CO]+
[M+H-3CH3OH-2CO]+
[M+H-2CH3OH-CO-H2O]+
[M+H-3CH3OH-2CO-H2O]+
522.0
[M+H-2CH3OH-CO]+
354.1
480.0
512.1
508.0
[M+H-CH3OH-H2O]+
462.0
490.2
540.1
582.1
Intensity, cps
m/z, Da


BMA
[M+H]+ 590.2
[M+H-CH3OH-H2O]+
540.1
[M+H-2CH3OH-H2O]+
[M+H-3CH3OH]+
[M+H-2CH3OH]+
[M+H-2CH3OH-2H2O]+
105.0
494.2
508.0
558.0 [M+H-CH3OH]+
490.1
572.2 [M+H-H2O]+
464.0
526.1
424.2
Intensity, cps
m/z, Da

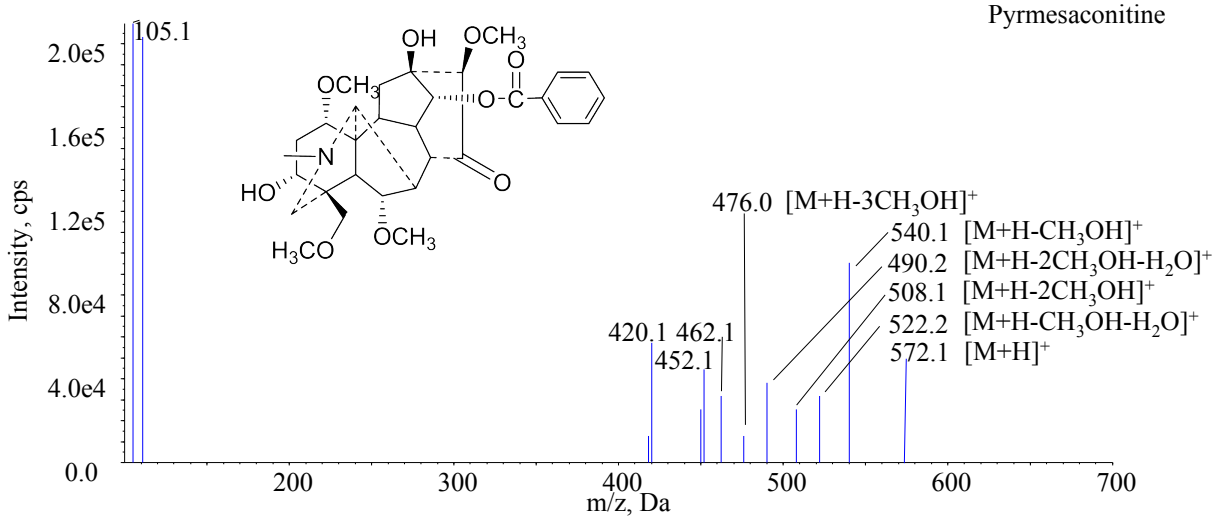

Pyrmesaconitine
105.1
476.0 [M+H-3CH3OH]+
540.1 [M+H-CH3OH]+
490.2 [M+H-2CH3OH-H2O]+
508.1 [M+H-2CH3OH]+
420.1 462.1
522.2 [M+H-CH3OH-H2O]+
452.1
572.1 [M+H]+
Intensity, cps
m/z, Da

Fig. S2

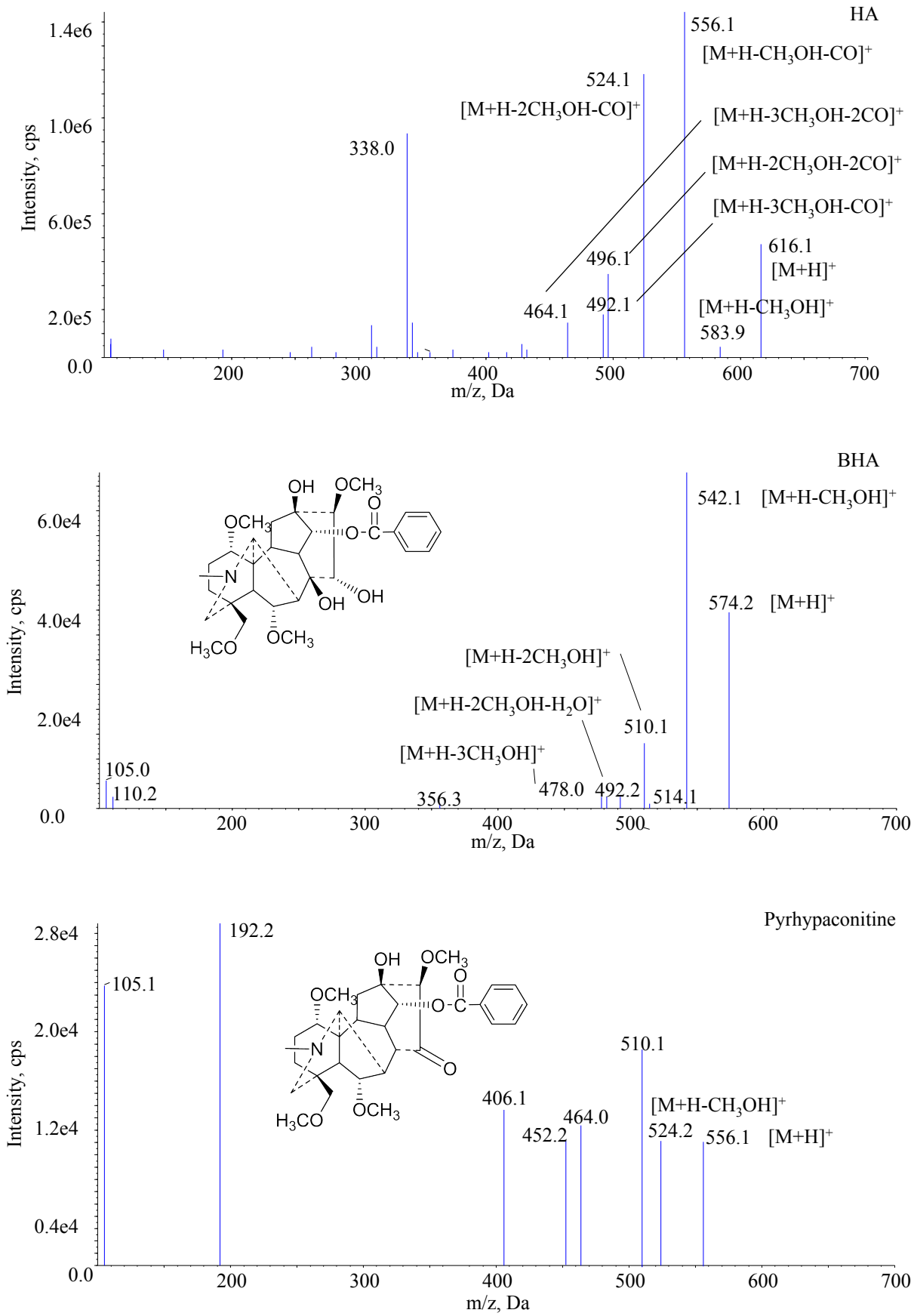

HA
556.1
[M+H-CH3OH-CO]+
524.1
[M+H-2CH3OH-CO]+
[M+H-3CH3OH-2CO]+
[M+H-2CH3OH-2CO]+
[M+H-3CH3OH-CO]+
338.0
496.1
616.1
[M+H]+
464.1
492.1
[M+H-CH3OH]+
583.9
Intensity, cps
m/z, Da
BHA
542.1 [M+H-CH3OH]+
574.2 [M+H]+
[M+H-2CH3OH]+
[M+H-2CH3OH-H2O]+
510.1
[M+H-3CH3OH]+
105.0
110.2
356.3
478.0
492.2
514.1
Pyrhypaconitine
192.2
105.1
510.1
406.1
464.0
452.2
[M+H-CH3OH]+
524.2
556.1
[M+H]+

Fig. S3