Electronic Supplementary Material (ESI) for Analytical Methods
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UPLC-Q-TOF/MS Characterization, HPLC Fingerprint Analysis and Species Differentiation for Quality Control of *Nigella glandulifera* Freyn et Sint Seeds and *Nigella sativa* L. Seeds

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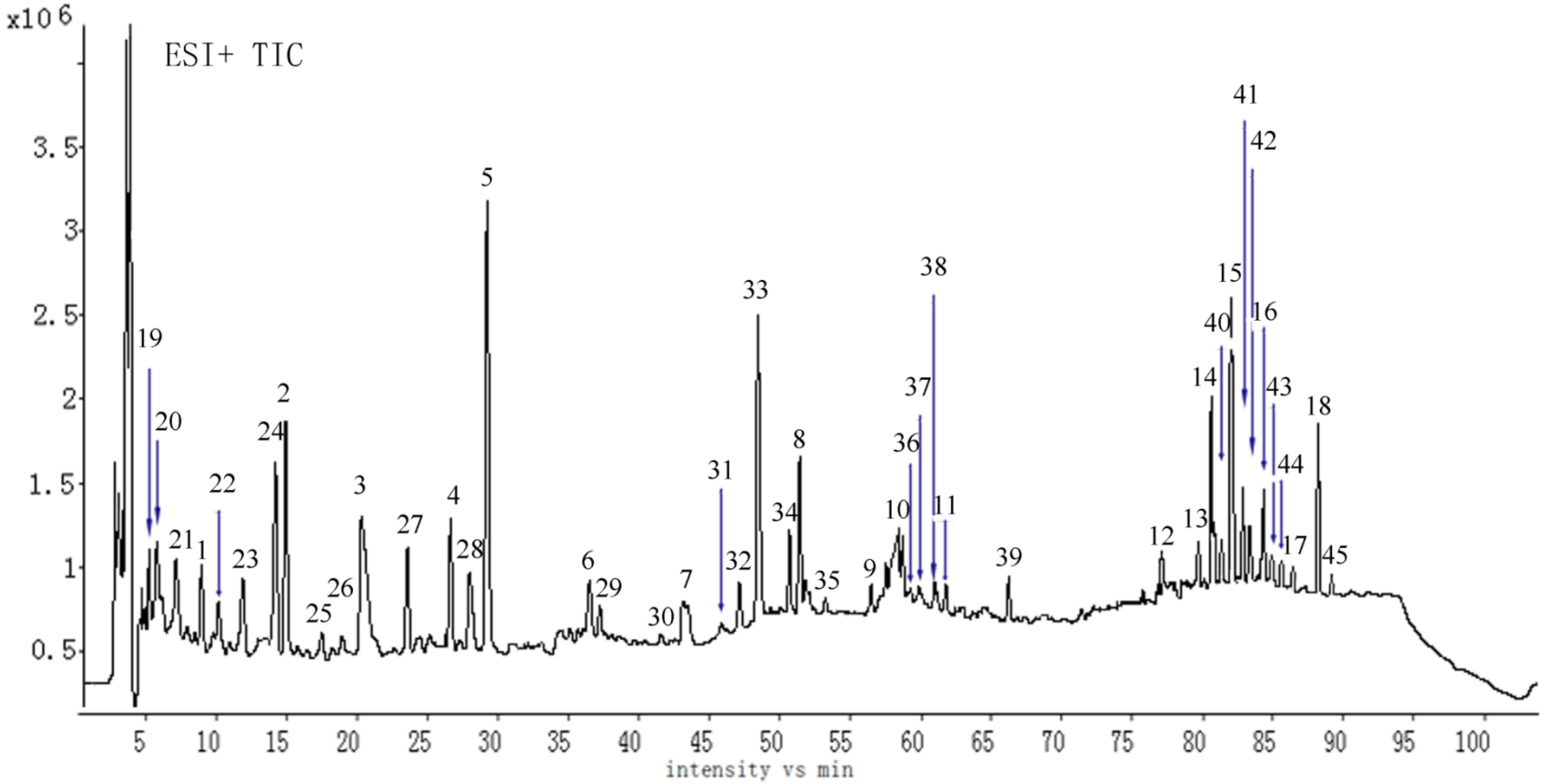
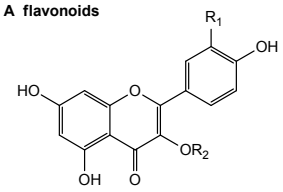


Fig. S1 The TIC chromatogram of NG in positive ion mode.

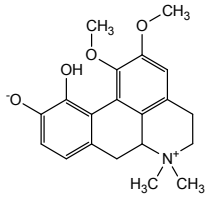
A flavonoids



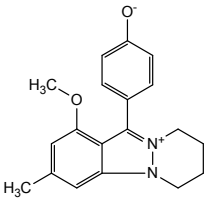
No	Name	R_1	R_2
4	Nigelflavonoside B	OH	β-D-glu(1→2)-β-D-gal-(1→2)-[6-α-L-rha(1→6)]-β-D-glu(1→3)
5	Quercetin-3-sophorotrioside	OH	β-D-glu(1→2)-β-D-glu(1→2)-β-D-glu(1→3)
6	Nigelloside	H	α-L-rha(1→6)-β-D-gal(1→3)-β-D-glu(1→3)-β-D-glu(1→3)
7	Nigeglanoside	H	β-D-gal(1→3)-β-D-glu(1→3)-β-D-glu(1→3)
31	Kaempferide	H	H

gal: -D-galactopyranosyl; glu: -D-glucopyranosyl; rha: -L-rhamnopyranosyl

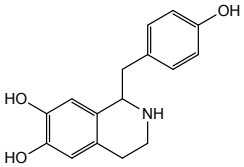
B alkaloids



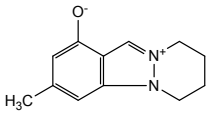
3. Fuzitinechloride



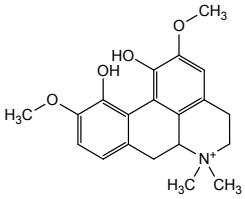
8. Methyl nigellidine



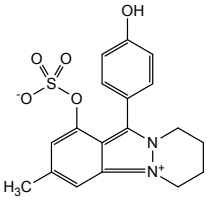
24. Higenamine



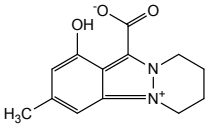
25. Nigeglanine



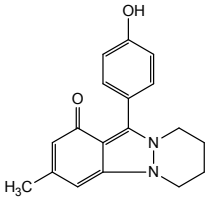
27. Magnoflorine



28. Nigellidine-4-o-sulfite

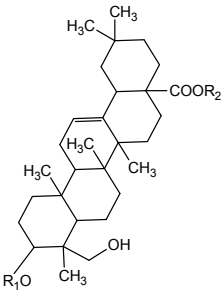


29. Nigellicine



33. Nigellidine

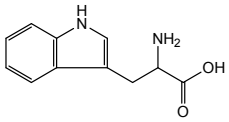
C hederagenin glycosides



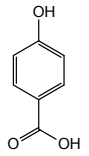
No	Name	R_1	R_2
13	Sieboldianoside A	β-D-xyl(1→3)-α-L-rha(1→2)-α-L-ara(1→3)	α-L-rha(1→4)-β-D-glu(1→6)-β-D-glu(1→28)
14	Tauroside H2	α-L-rha(1→2)-α-L-ara(1→3)	α-L-rha(1→4)-β-D-glu(1→6)-β-D-glu(1→28)
15	Tauroside G3	α-L-rha(1→2)-α-L-ara(1→3)	β-D-glu(1→6)-β-D-glu(1→28)
16	3-O-[β-D-xylopyranosyl-(1→3)-α-l-rhamnopyranosyl-(1→4)-β-D-glucopyranosyl]-11-methoxy-16-hydroxy-17-acetoxy hederagenin	β-D-xyl-(1→3)-α-l-rha-(1→4)-β-D-glu(1→3)	CH_3
17	Sapindoside B	β-D-xyl(1→3)-α-L-rha(1→2)-α-L-ara（1→3）	H
18/45	Tauroside E	α-L-rha(1→2)-α-L-ara(1→3)	H
40	Decaisoside E	β-D-xyl(1→3)-α-L-rha(1→2)-α-L-ara(1→3)	β-D-glu(1→6)-β-D-glu(1→28)
42	Decaisoside D	β-D-xyl(1→3)-α-L-rha(1→2)-α-L-ara(1→3)	β-D-glu(1→28)

ara: -L-arabinopyranosyl; glu: -D-glucopyranosyl; rha: -L-rhamnopyranosyl; xyl: -D-xylopyranosyl

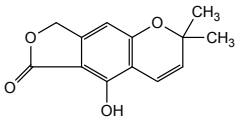
D other types



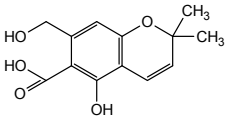
1. L-Tryptophan



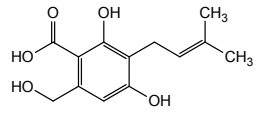
2. *p*-Hydroxybenzoic acid



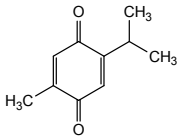
9. Salfredin B_{11}



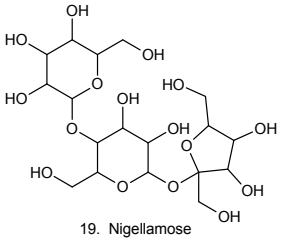
10. Hydrate salfredin B_{11}



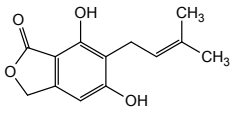
11. 2,4-dihydroxy-6-(hydroxymethyl)-3-(3-methylbut-2-enyl)benzoic acid



12. Thymoquinone



19. Nigellamose



38. 5,7-dihydroxy-6-(3-methybut-2-enyl) isobenzofuran-1(3H)-one

Fig. S2 Chemical structures of the identified compounds in NG and NS.

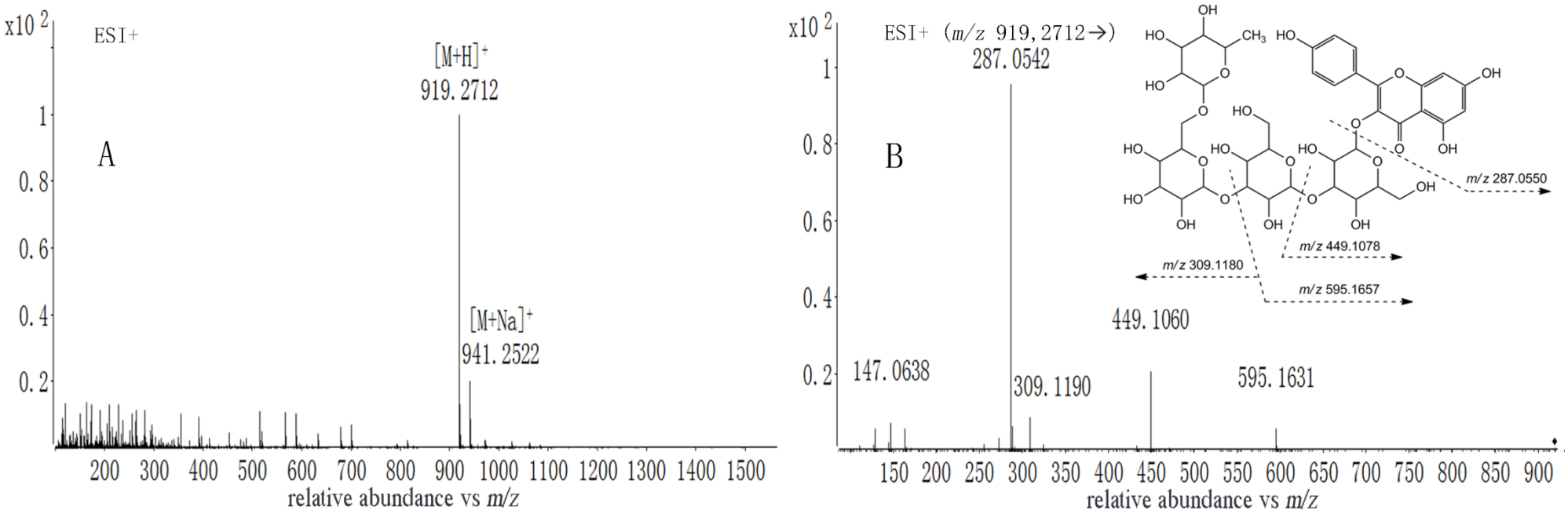


Fig. S3 MS spectrum (A) and MS^2 spectrum for m/z 919.2712 (B) of peak6 (nigelloside) in positive mode.

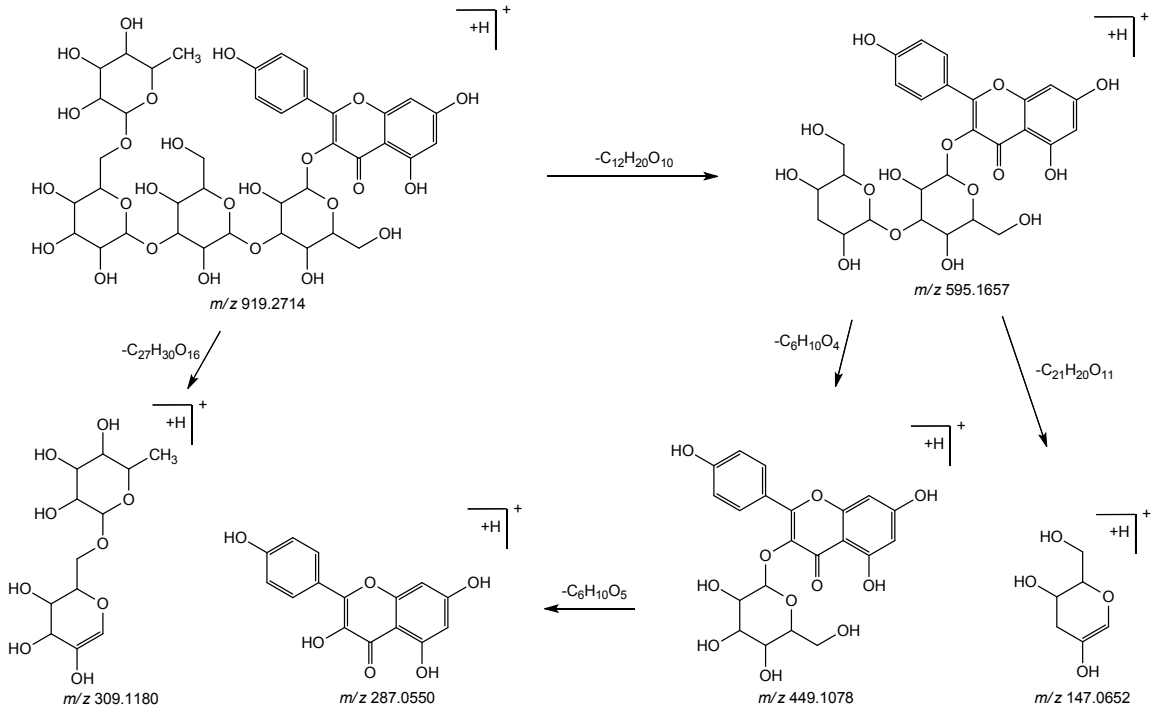


Fig. S4 Proposed fragmentation pathway of peak6 (nigelloside) in positive mode.

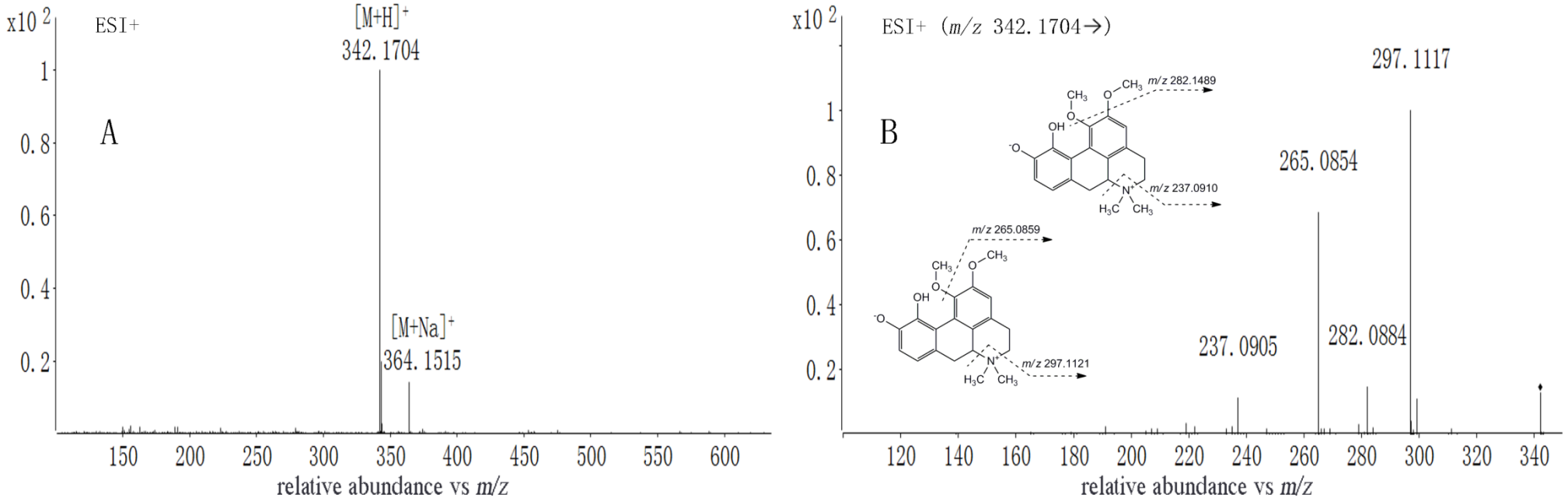


Fig. S5 MS spectrum (A) and MS^2 spectrum for *m/z* 342.1704 (B) of peak3 (fuzitinechloride) in positive mode.

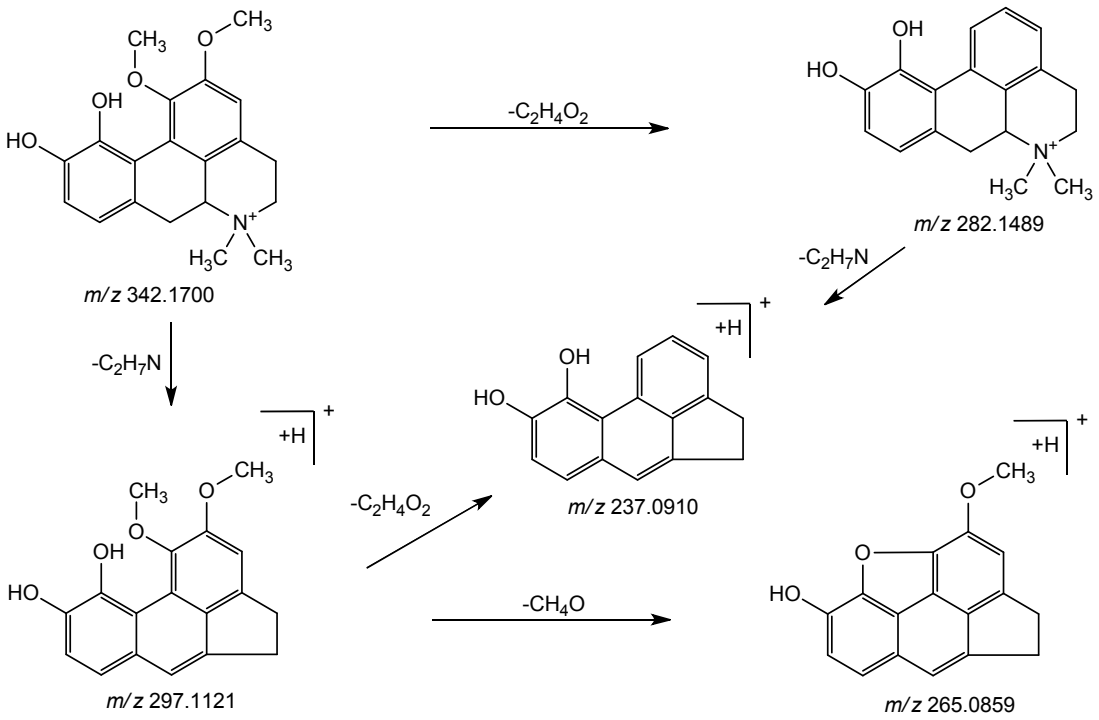


Fig. S6 Proposed fragmentation pathway of peak3 (fuzitinechloride) in positive mode.

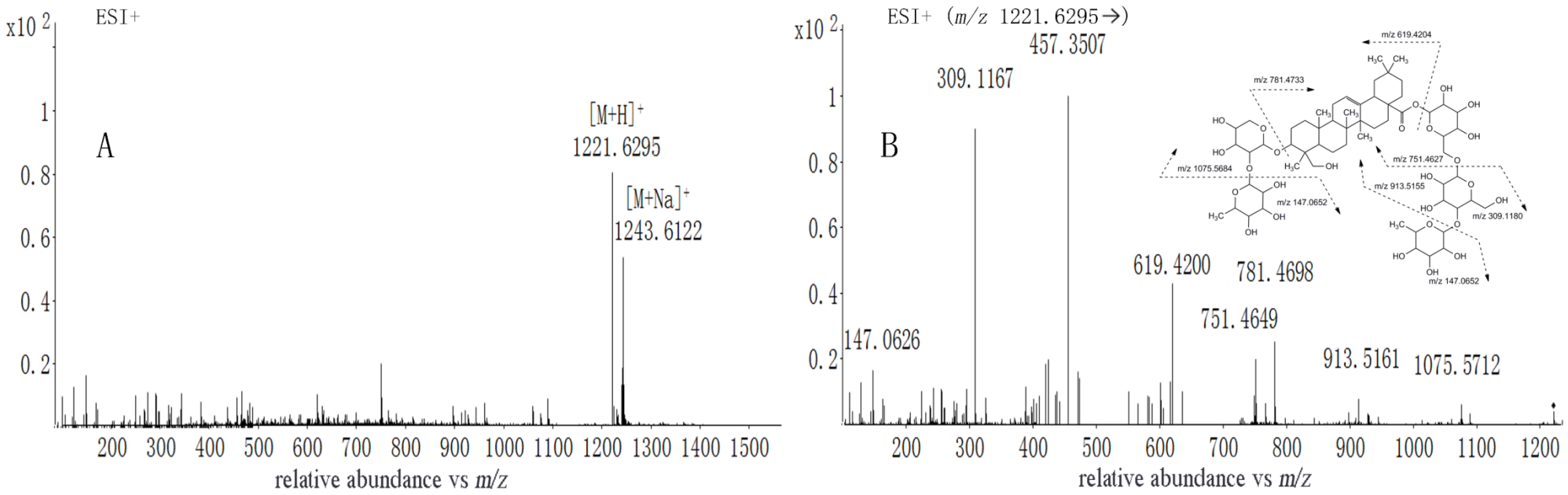


Fig. S7 MS spectrum (A) and MS^2 spectrum for *m/z* 1221.6295 (B) of peak14 (tauroside H2) in positive mode.

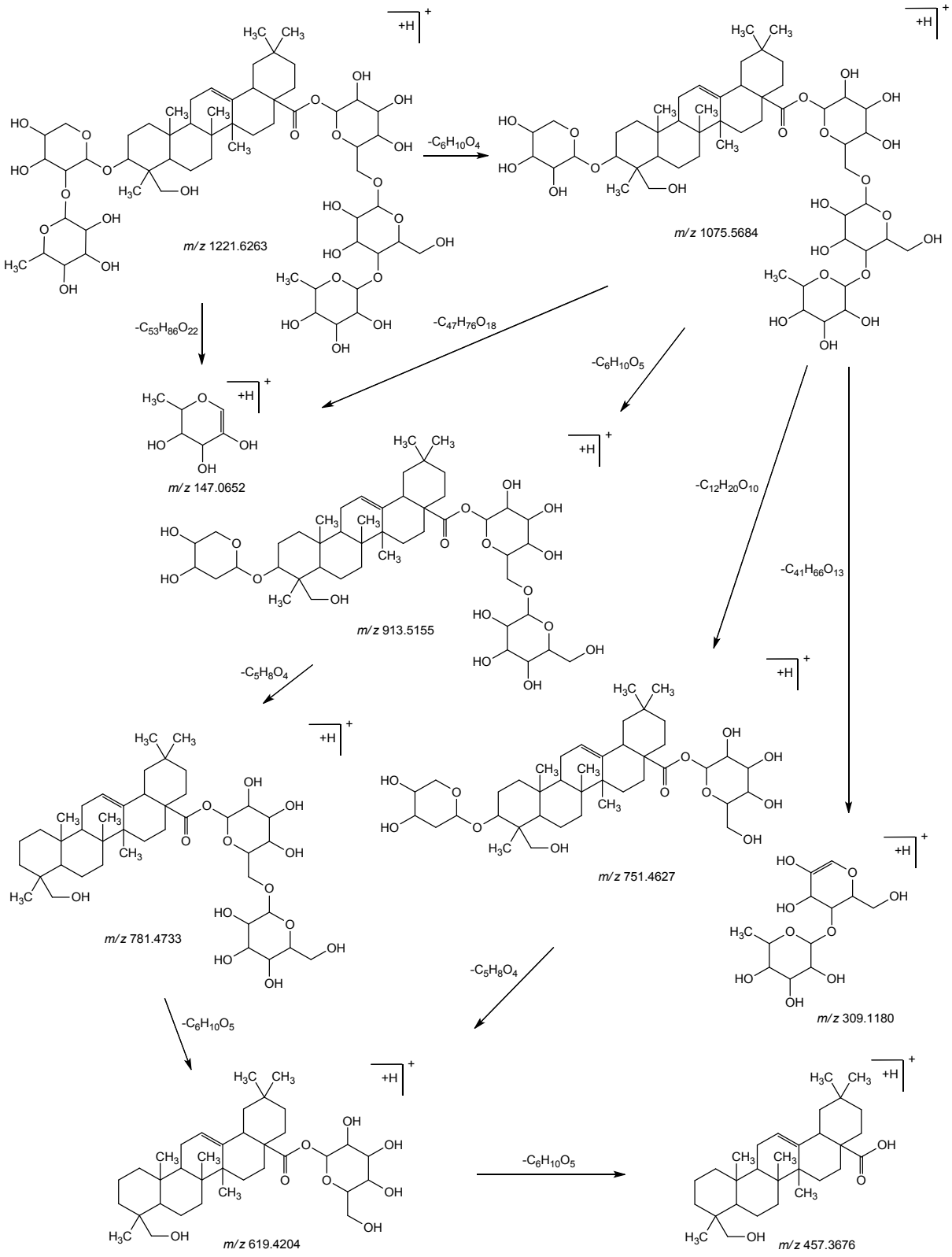


Fig. S8 Proposed fragmentation pathway of peak14 (tauroside H2) in positive mode.