molecules

MDPI

Supplementary Materials

Identification of Polar Constituents in the Decoction of *Juglans mandshurica* and in the Medicated Egg Decocted with the Decoction by HPLC-Q-TOF MS²

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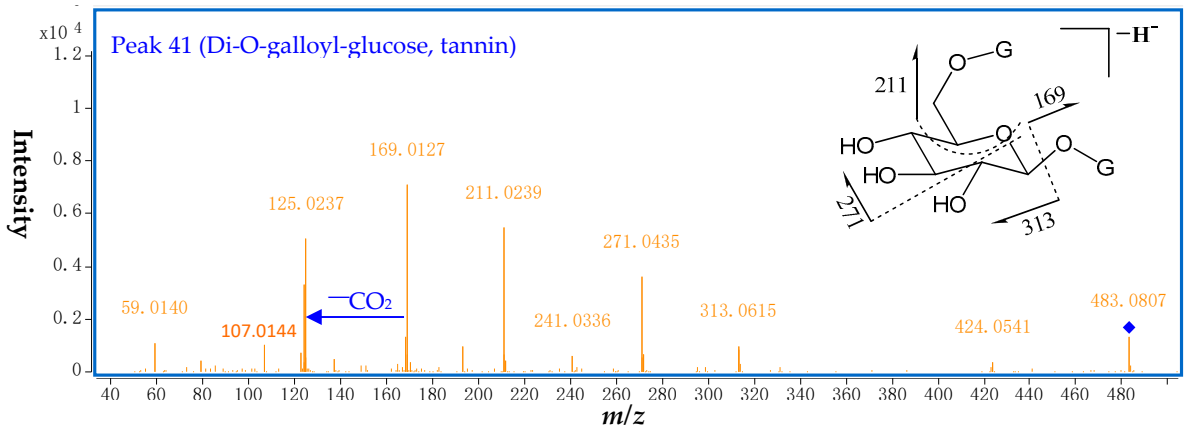
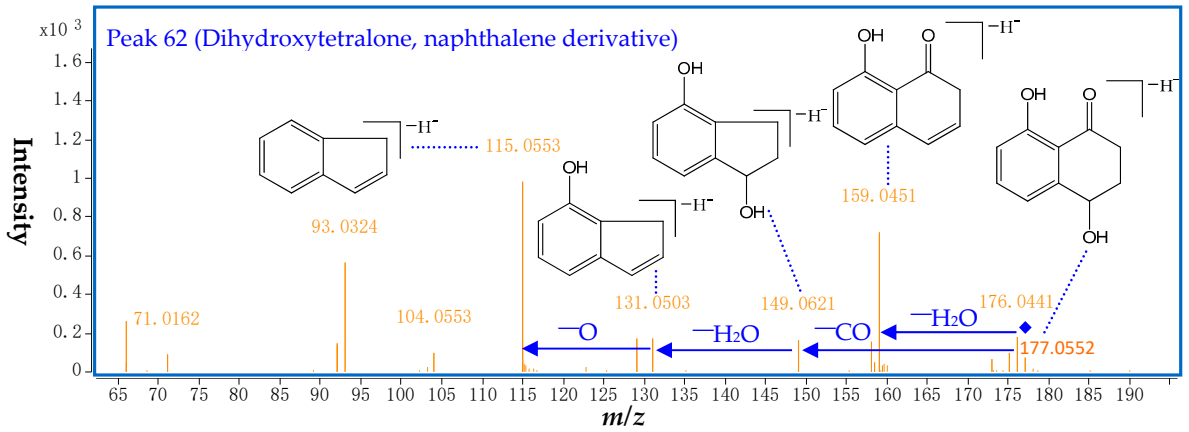
Table S1 Information for reference compounds.

No.	Reference compound	Structural type	Concentration (μg/mL)	Standard solution	t_R (min)
1	Gallic acid	Organic acid	21	A	7.9
2	Protocatechuic acid	Organic acid	36	A	13.1
3	Chlorogenic acid	Organic acid	22	A	19.5
4	Caffeic acid	Organic acid	15	B	21.8
5	Syringic acid	Organic acid	15	A	22.6
6	1,2,6-Tri-O-galloyl-*β*-D-glucose	Tannin	35	A	22.7
7	1,4,8-Trihydroxy-naphthalene-1-O-*β*-D-glucoside	Naphthalene	35	A	24.4
8	*p*-Coumaric acid	Organic acid	25	B	27.5
9	1,2,3,6-Tetra-O-galloyl-*β*-D-glucose	Tannin	35	A	29.2
10	Rutin	Flavonoid	106	B	29.6
11	Ellagic acid	Organic acid	10	B	30.0
12	Sinapic acid	Organic acid	20	B	30.3
13	Quercetin-3-O-*α*-L-rhamnoside	Flavonoid	56	A	34.2
14	Kaempferol-3-O-*α*-L-rhamnoside	Flavonoid	56	A	37.9
15	Luteolin	Flavonoid	116	B	42.4
16	Quercetin	Flavonoid	70	A	42.6
17	Juglone	Naphthoquinone	45	A	43.9
18	Apigenin	Flavonoid	62	B/A	45.6
19	Kaempferol	Flavonoid	98	A/B	46.2
20	Acacetin	Flavonoid	110	A	52.8

(a)



(b)



(c)

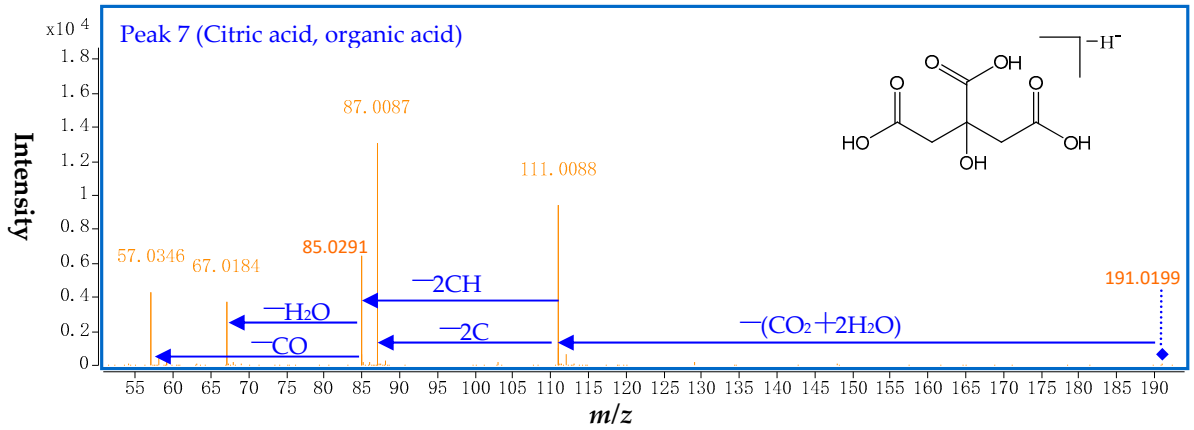
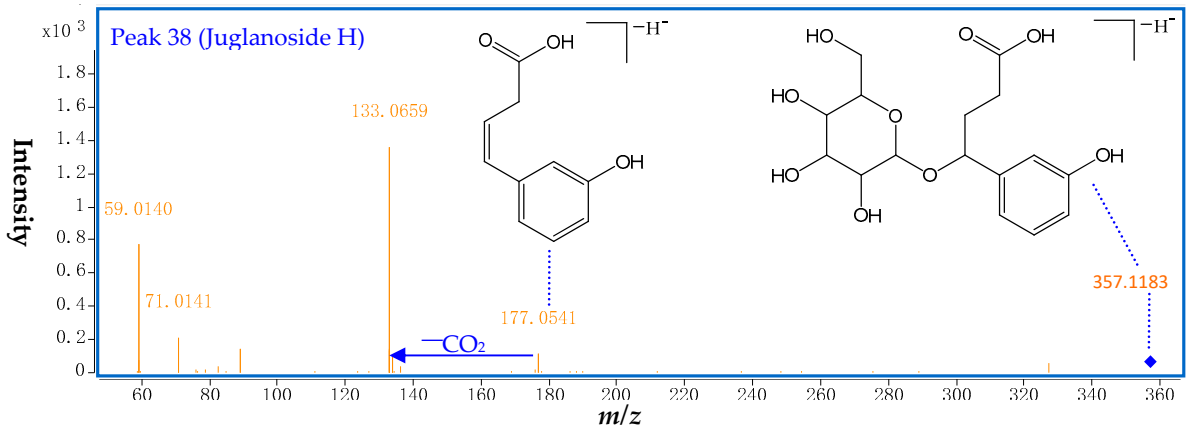
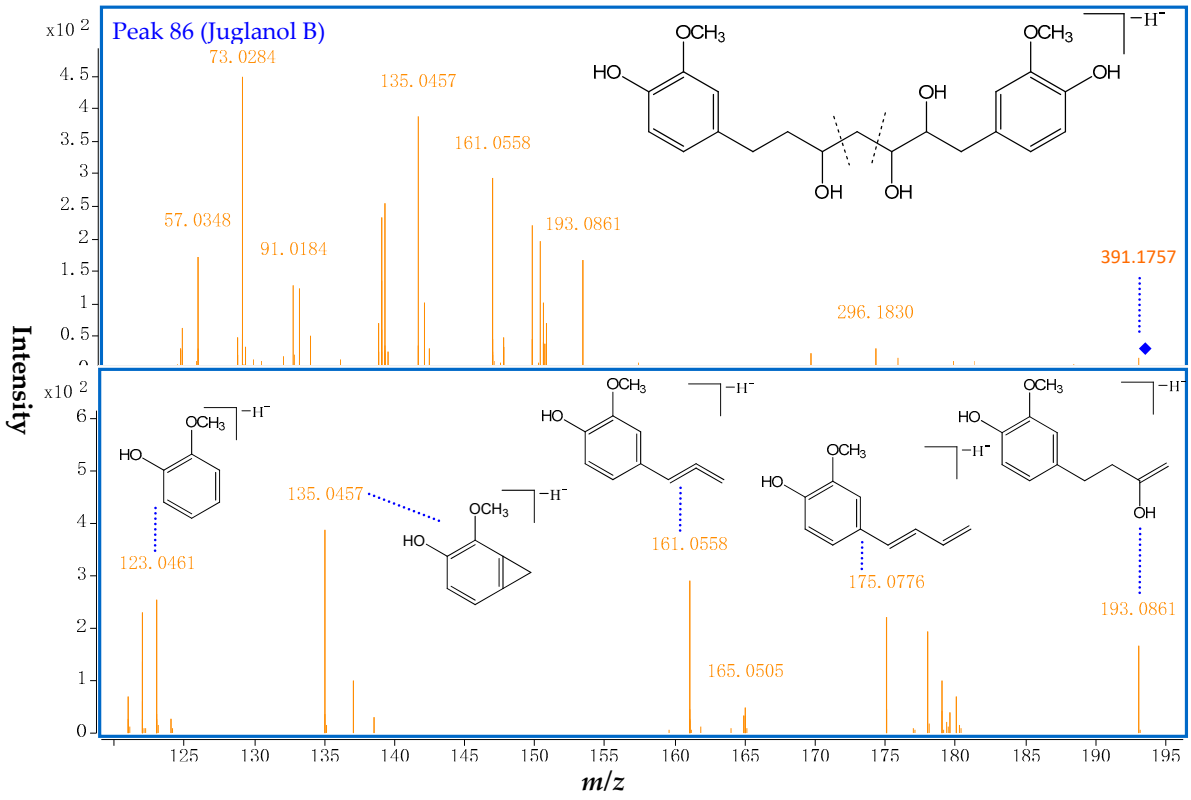


Figure S1 Representation of the fragmentation pattern of (**a**) tannins (Peak 41), (**b**) naphthalene derivatives (Peak 62) and (**c**) organic acids (Peak 7).

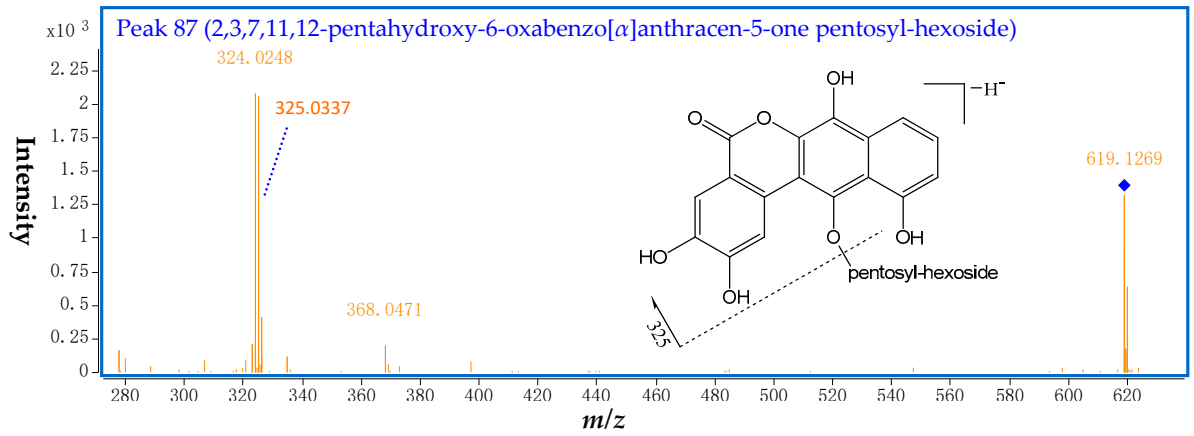
(a)


Peak 38 (Juglanoside H)
Intensity
m/z
133. 0659
59. 0140
71. 0141
177. 0541
357.1183
−CO2
−H-

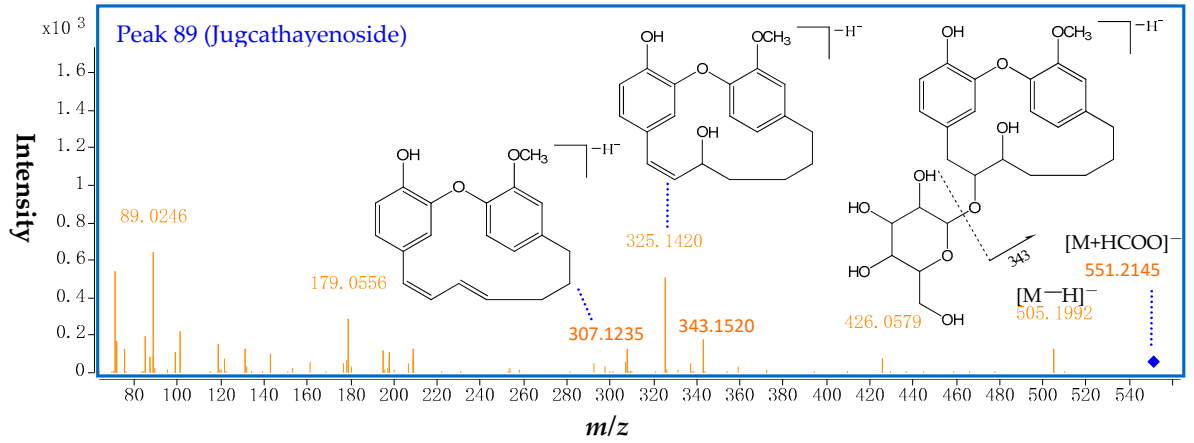
(b)


Peak 86 (Juglanol B)
Intensity
m/z
73. 0284
135. 0457
161. 0558
57. 0348
91. 0184
193. 0861
296. 1830
391.1757
123. 0461
165. 0505
175. 0776
−H-

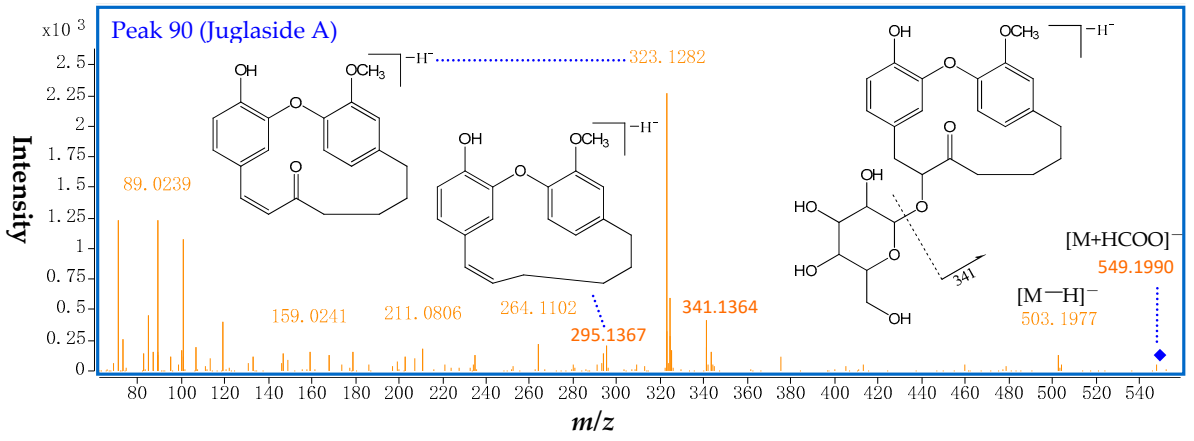
(c)


Peak 87 (2,3,7,11,12-pentahydroxy-6-oxabenzo[α]anthracen-5-one pentosyl-hexoside)
x10 3
Intensity
324. 0248
325.0337
368. 0471
619. 1269
pentosyl-hexoside
m/z

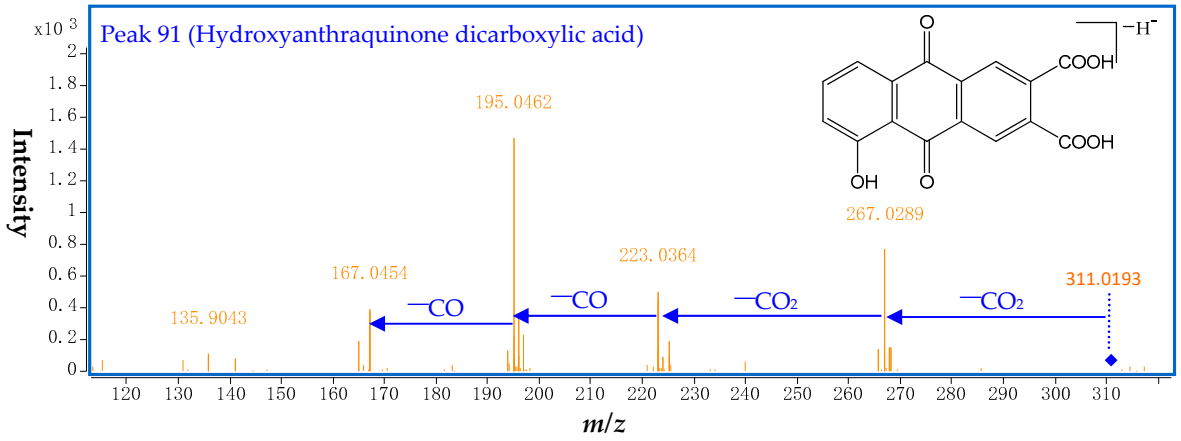
(d)


Peak 89 (Jugcathayenoside)
x10 3
Intensity
89. 0246
179. 0556
307.1235
325. 1420
343.1520
426. 0579
[M+HCOO]⁻
551.2145
[M—H]⁻
505. 1992
m/z

(e)


Peak 90 (Juglaside A)
x10 3
Intensity
89. 0239
159. 0241
211. 0806
264. 1102
295.1367
323. 1282
341.1364
[M+HCOO]⁻
549.1990
[M—H]⁻
503. 1977
m/z

(f)



(g)

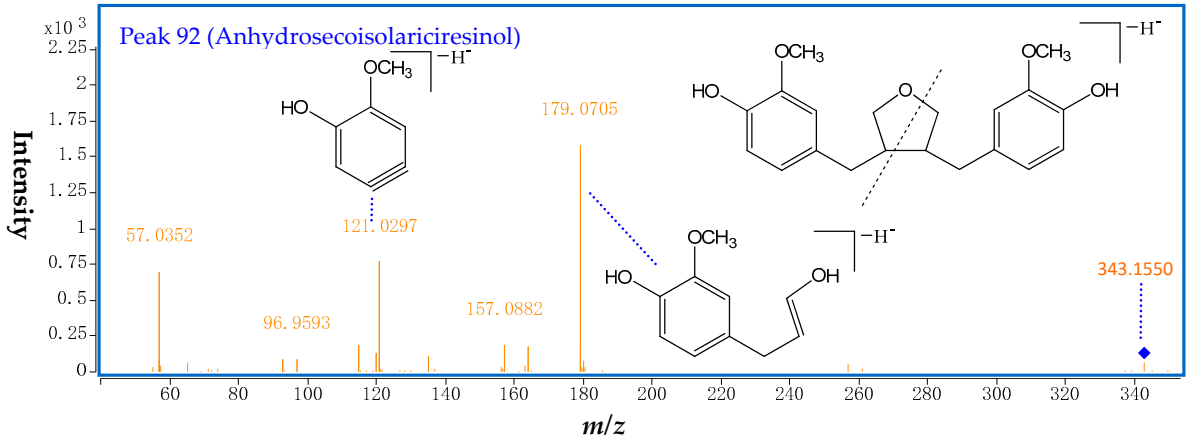
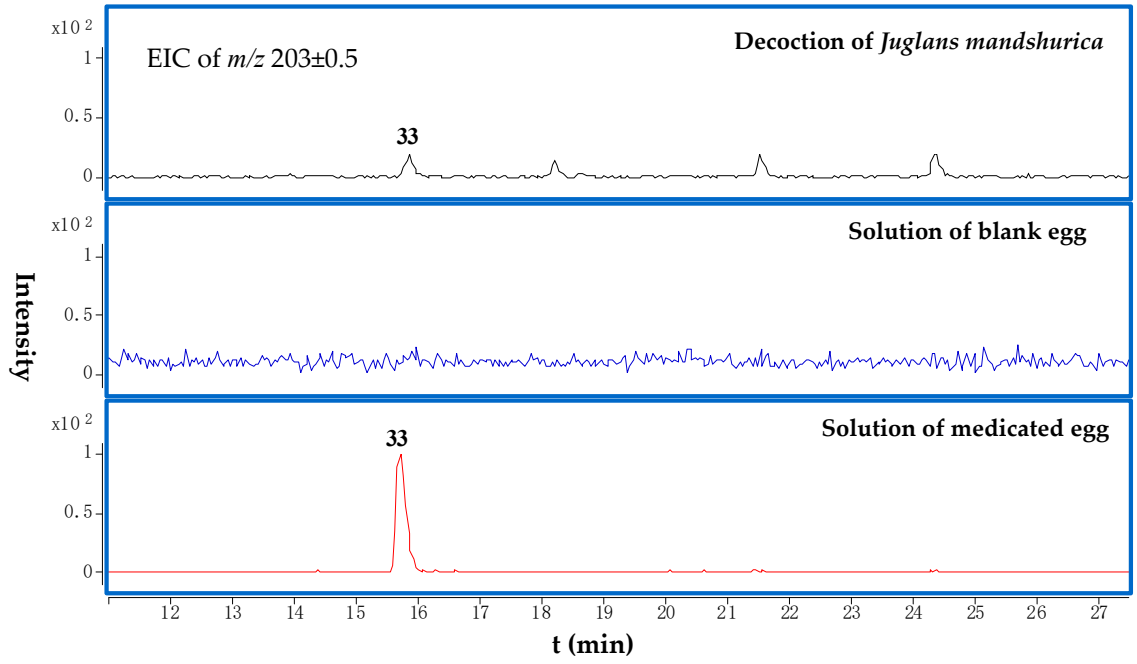


Figure S2 Proposed fragmentation pattern of the compounds tentatively identified: (**a**) Peak 38, (**b**) Peak 86, (**c**) Peak 87, (**d**) Peak 89, (**e**) Peak 90, (**f**) Peak 91 and (**g**) Peak 92.

(a)



(b)

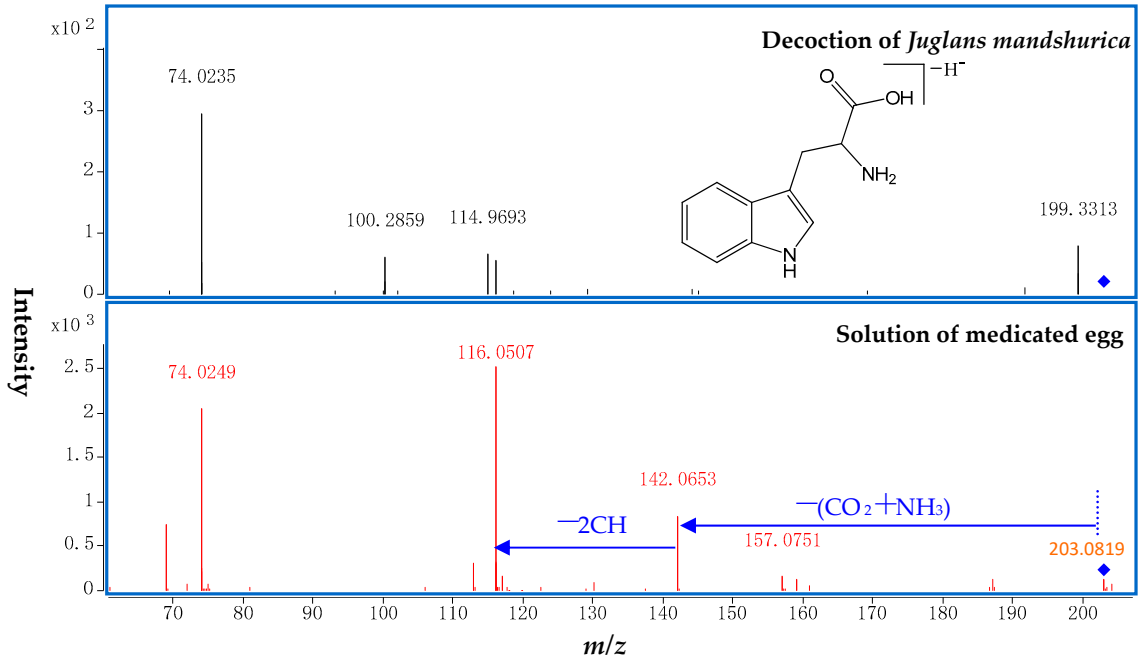


Figure S3 (**a**) EIC of the *Juglans mandshurica* decoction and blank and medicated egg solutions at *m*/*z* 203 in MS and (**b**) CID MS/MS spectra (obtained at an energy of −20 eV) of the ion at *m*/*z* 203±0.5 in the *Juglans mandshurica* decoction and medicated egg solution. Peak 33 was identified as tryptophan.

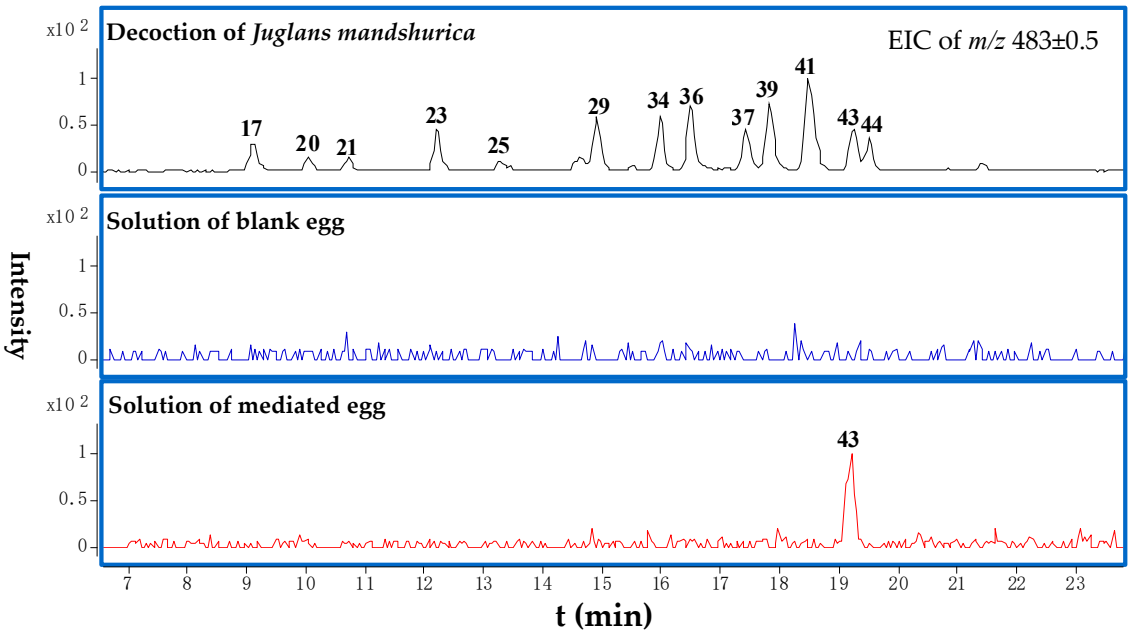


Figure S4 EIC of the *Juglans mandshurica* decoction and blank and medicated egg solutions at *m/z* 483±0.5 in MS. Peaks 43 was identified as hydroxy-dimethoxyphenol galloyl-glucoside, and other peaks were identified as isomers of di-O-galloyl-glucose.