Exploring potential quality markers of Paeoniae Radix Alba by UPLC-Q-TOF/MS, HPLC, and cell experimentation

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SUPPORTING INFORMATION

Fig. S1 Speculated fragmentation pathways of compound 39.

Fig. S2 Speculated fragmentation pathways of compound 47.

Fig. S3 Speculated fragmentation pathways of compound 26.

Fig. S4 Speculated fragmentation pathways of compound 16.

Fig. S5 Speculated fragmentation pathways of compound 4.

Fig. S6 Heat map analysis of 13 common peaks in the 12 batches of PRA.

Fig. S7 HPLC chromatograms of mixed standard (A), sample (B), and blank solvent (C). 1: Oxypaeoniflorin; 2: Albiflorin; 3: Paeoniflorin; 4: Lactiflorin; 5: Palbinone.

Fig. S8 Effects of albiflorin (A), oxypaeoniflorin (B), lactiflorin (C), paeoniflorin (D), and palbinone (E) on cell viability. $^*p < 0.05$ and $^{**}p < 0.01$ vs. control group; All data

were expressed as mean ± SD.

Table S1 The information of PRA.

Table S2 The results of precision, repeatability, and stability tests in the fingerprint analysis.

Table S3 The results of precision, repeatability, stability, and recovery tests in the quantitative analysis

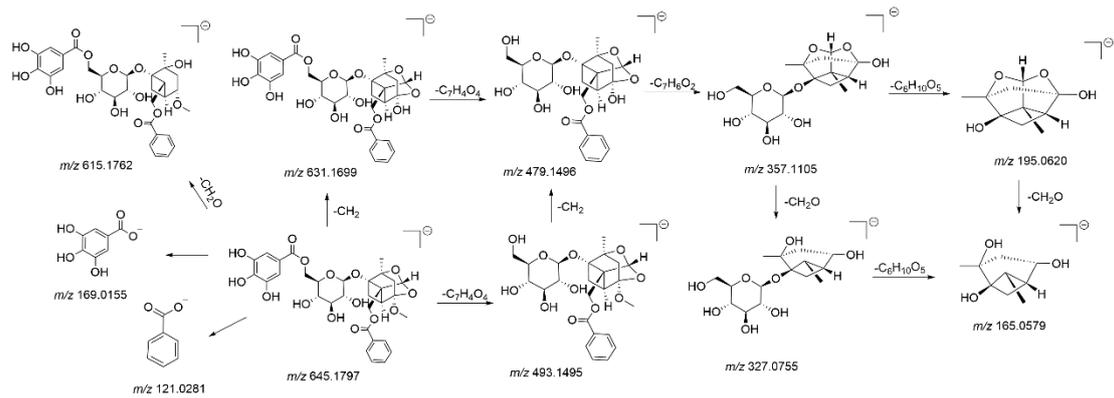Table S4 Contents of five potential active compounds in 12 batches of PRA samples $(mg\ g^{-1}, n = 3)$.
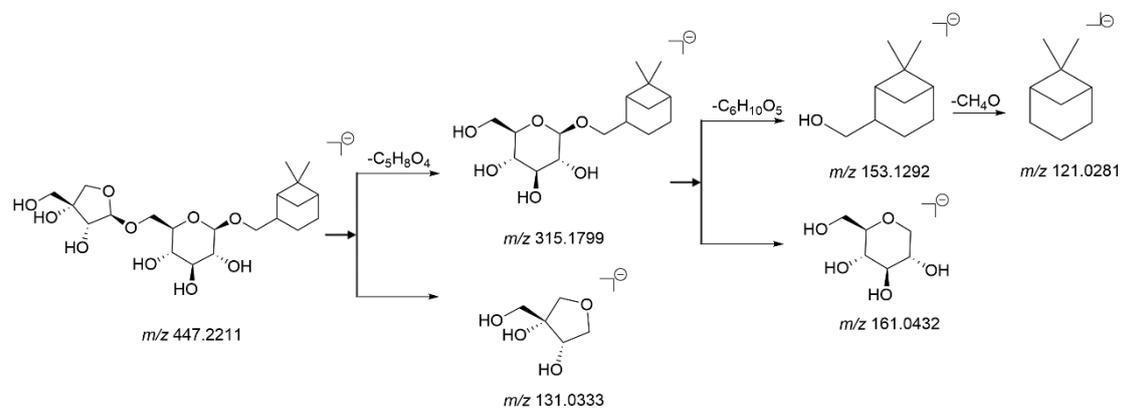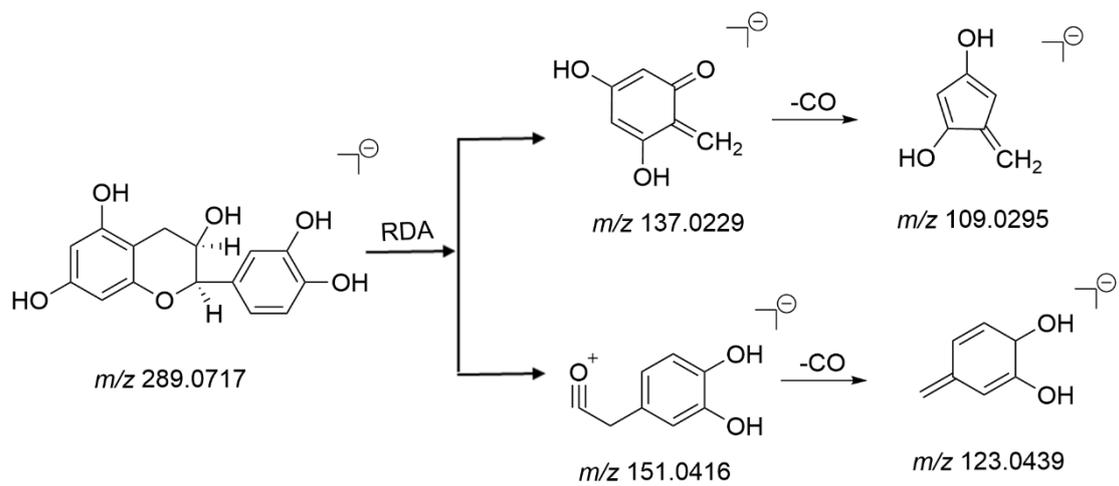
Fig. S1

Fig. S2

Fig. S3

Fig. S4

m/z 493.1216   -$C_6H_{10}O_5$ *m/z* 331.0661   -$C_6H_{10}O_5$ *m/z* 169.0155

-H_2O *m/z* 313.0526

-CO_2 *m/z* 125.0219

-H_2O *m/z* 107.0128
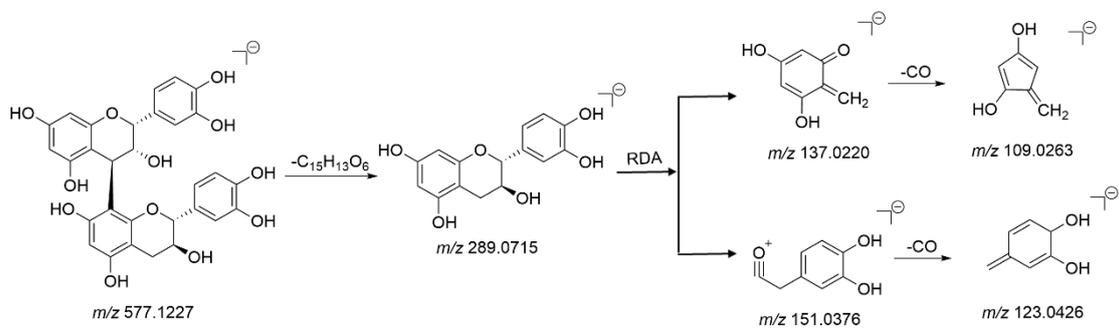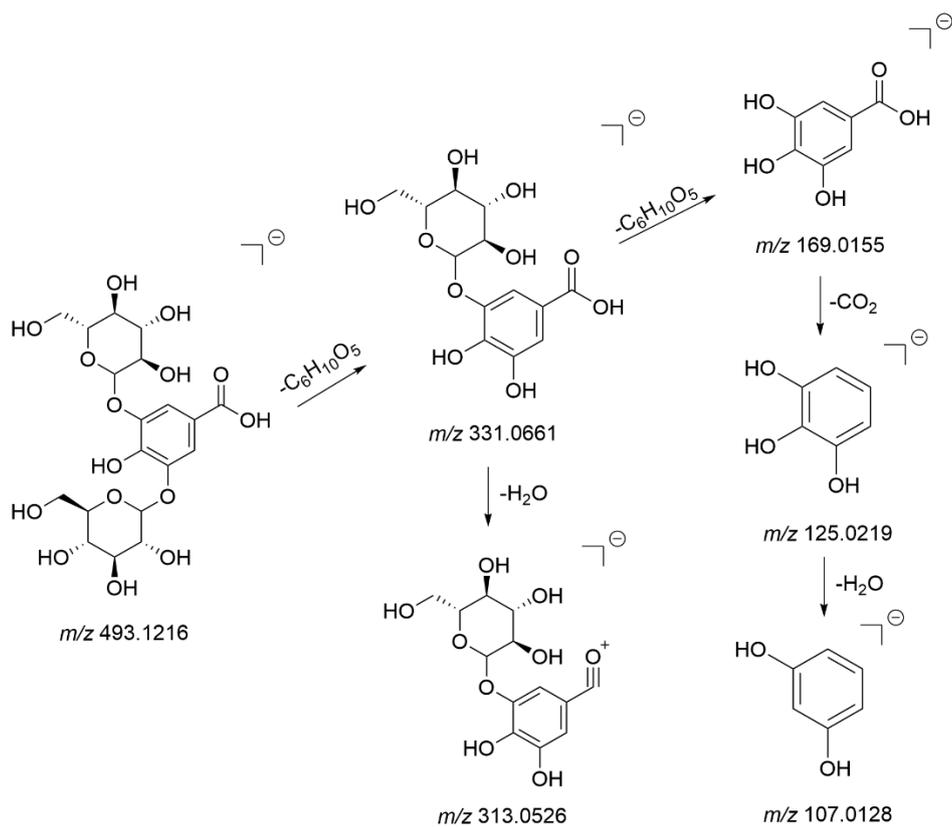
Fig. S5
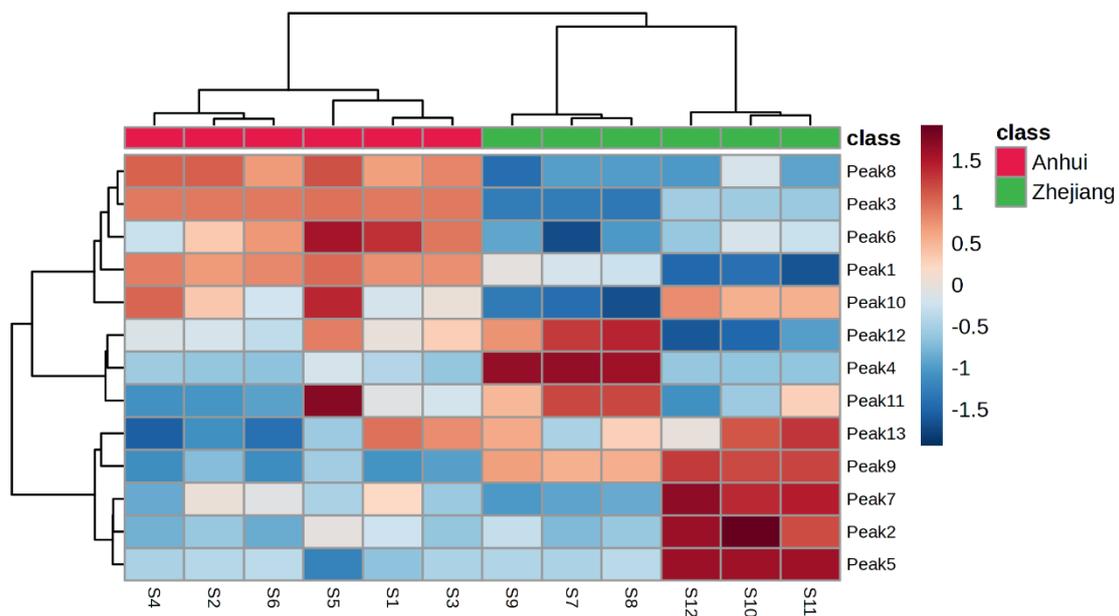
Fig. S6
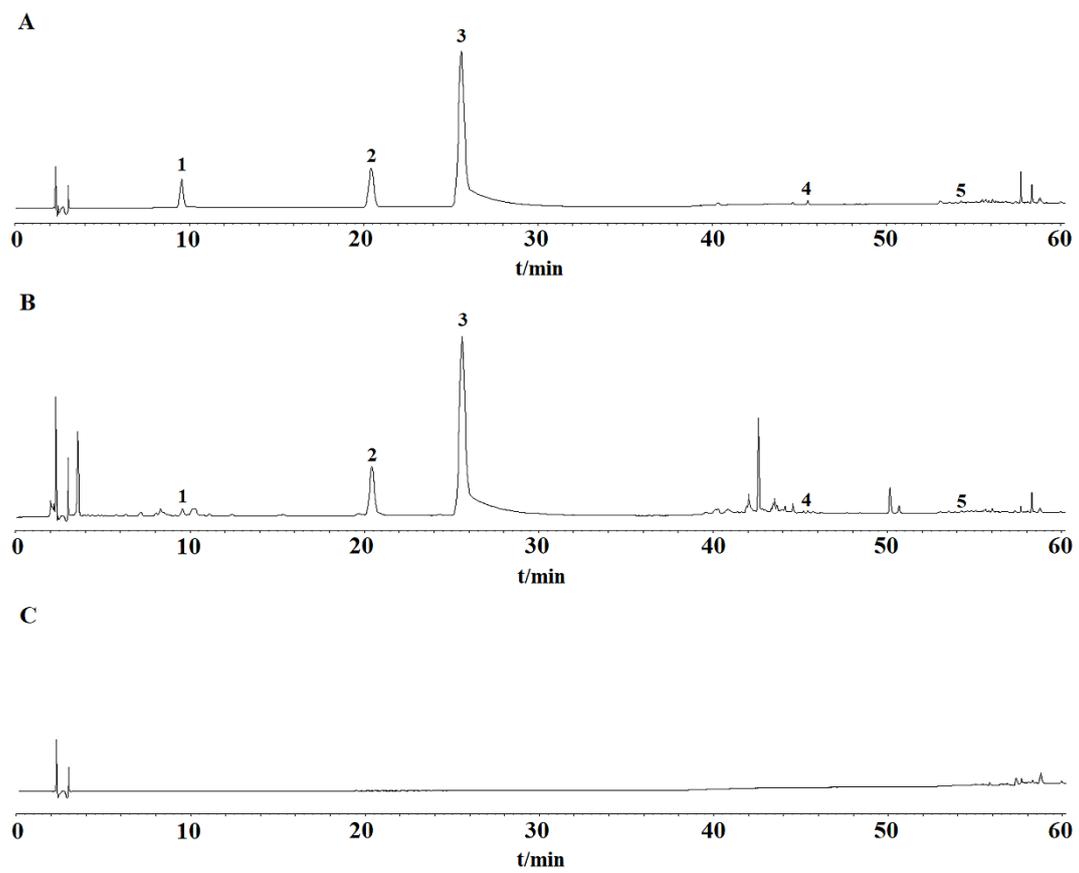
Fig. S7
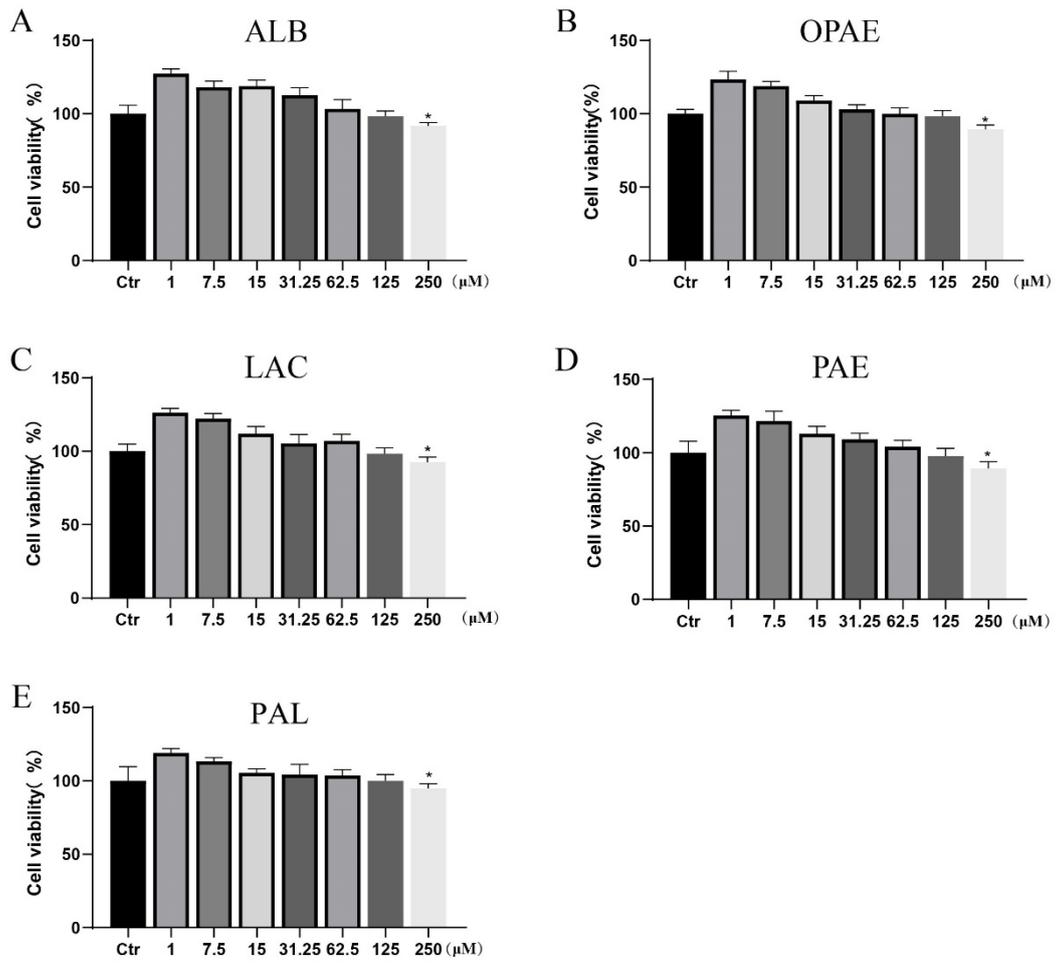
Fig. S8

Table S1 The information of PRA.

Batch	Original place	Purchase channel	Batch number
S1	Shibali Town, Qiaocheng District, Bozhou City, Anhui Province, China	Beijing Tongrentang Drug Store	2022052701
S2	Shibali Town, Qiaocheng District, Bozhou City, Anhui Province, China	Beijing Tongrentang Drug Store	2022080101
S3	Shibali Town, Qiaocheng District, Bozhou City, Anhui Province, China	Beijing Tongrentang Drug Store	2022111001
S4	Shijiuli Town, Qiaocheng District, Bozhou City, Anhui Province, China	Dongjitang Pharmaceutical Co., Ltd	221101
S5	Shijiuli Town, Qiaocheng District, Bozhou City, Anhui Province, China	Dongjitang Pharmaceutical Co., Ltd	220901
S6	Shijiuli Town, Qiaocheng District, Bozhou City, Anhui Province, China	Dongjitang Pharmaceutical Co., Ltd	220601
S7	Panan County, Jinhua City, Zhejiang Province, China	Hebei Chufeng Chinese Medicine Herb in Pieces Co., Ltd	B22102201-01
S8	Panan County, Jinhua City, Zhejiang Province, China	Hebei Chufeng Chinese Medicine Herb in Pieces Co., Ltd	B22122401-01
S9	Panan County, Jinhua City, Zhejiang Province, China	Hebei Chufeng Chinese Medicine Herb in Pieces Co., Ltd	B23022201-01
S10	Panan County, Jinhua City, Zhejiang Province, China	Third Affiliated Hospital of Zhejiang University of Chinese Medicine	20220501
S11	Panan County, Jinhua City, Zhejiang Province, China	Third Affiliated Hospital of Zhejiang University of Chinese Medicine	20221003
S12	Panan County, Jinhua City, Zhejiang Province, China	Third Affiliated Hospital of Zhejiang University of Chinese Medicine	20230101

Table S2 The results of precision, repeatability, and stability tests in the fingerprint analysis.

Peak No.	%RSDs of RRT			%RSDs of RPA		
	Precision (n = 6)	Repeatability (n = 6)	Stability	Precision (n = 6)	Repeatability (n = 6)	Stability
1	0.23	0.22	0.14	0.85	1.90	1.30
2	0.20	0.14	0.09	0.78	2.33	0.92
3	0.16	0.07	0.04	0.75	2.24	0.77
4	0.17	0.05	0.03	0.63	1.37	0.66
5	0.00	0.00	0.00	0.00	0.00	0.00
6	0.22	0.14	0.09	0.98	1.97	2.17
7	0.26	0.19	0.10	1.12	2.61	2.06
8	0.27	0.21	0.10	2.44	2.13	2.25
9	0.26	0.20	0.10	2.55	2.43	2.12
10	0.26	0.20	0.10	2.64	2.64	1.57
11	0.26	0.20	0.10	0.81	2.65	0.64
12	0.26	0.75	0.10	0.89	2.44	1.11
13	0.27	0.54	0.10	0.00	0.00	0.00

Table S3 The results of precision, repeatability, stability, and recovery tests in the quantitative analysis.

Components	Precision RSD (%)		Repeatability RSD (%) (n = 6)	Stability RSD (%)	Recovery (n = 6)	
	Intra-day (n = 6)	Inter-day (n = 6)			Recovery (%)	RSD (%)
Oxypaeoniflorin	0.38	2.30	2.50	1.12	93.99	1.92
Albiflorin	0.57	3.03	1.85	1.07	101.99	1.83
Paeoniflorin	1.27	2.90	1.69	0.34	104.10	2.03
Lactiflorin	2.52	2.57	2.94	1.78	88.14	0.88
Palbinone	1.16	2.33	2.43	2.75	110.41	1.78

Table S4 Contents of five potential active compounds in 12 batches of PRA samples (mg g^{-1}, n = 3).

Batch	Oxypaeoniflorin	Albiflorin	Paeoniflorin	Lactiflorin	Palbinone
S1	0.296	5.822	28.550	0.032	0.004
S2	0.295	5.772	28.253	0.037	0.002
S3	0.292	5.755	26.215	0.034	0.002
S4	0.288	5.808	28.474	0.036	0.002
S5	0.281	5.723	27.774	0.036	0.002
S6	0.287	5.688	28.286	0.032	0.002
S7	0.309	7.677	28.863	0.056	0.004
S8	0.303	7.679	29.010	0.056	0.005
S9	0.309	7.608	28.978	0.058	0.005
S10	0.366	6.284	32.753	0.092	0.006
S11	0.359	6.369	32.745	0.076	0.005
S12	0.384	6.606	33.599	0.082	0.006