

Supplementary Material

LC-MS/MS coupled with chemometric analysis as an approach for the differentiation of *Fritillariae cirrhosae* bulbus and *Fritillariae pallidiflorae* bulbus

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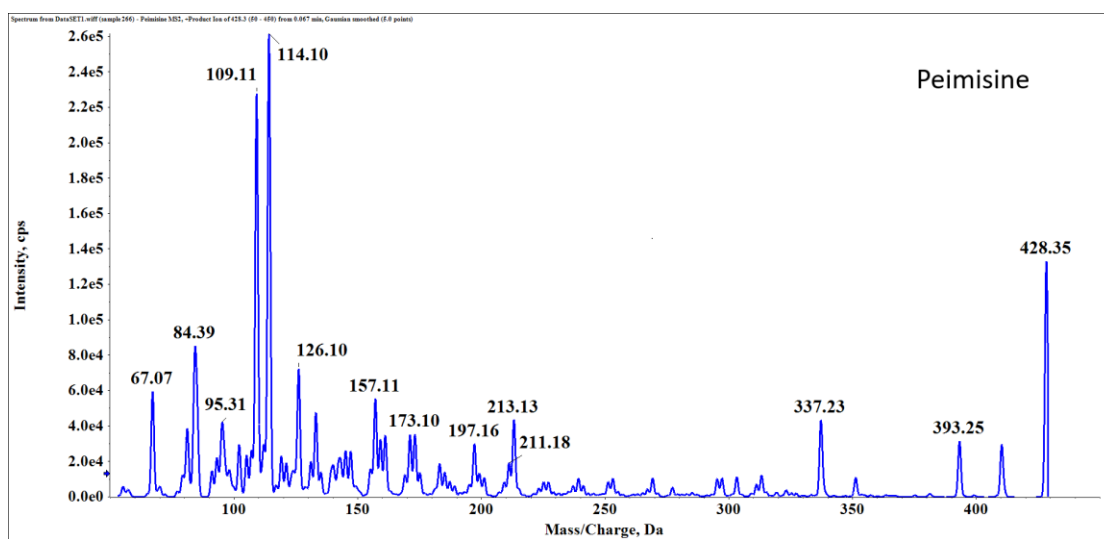
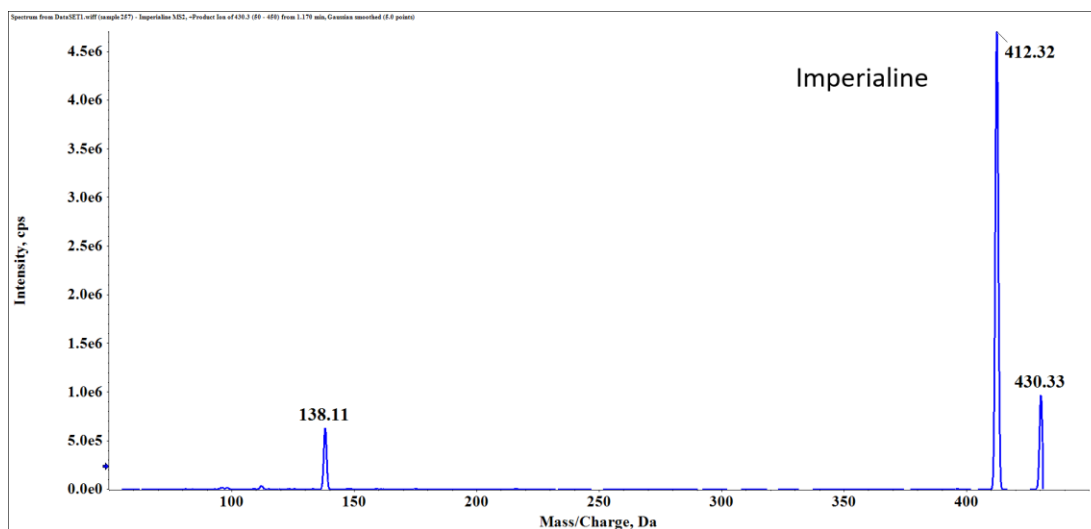
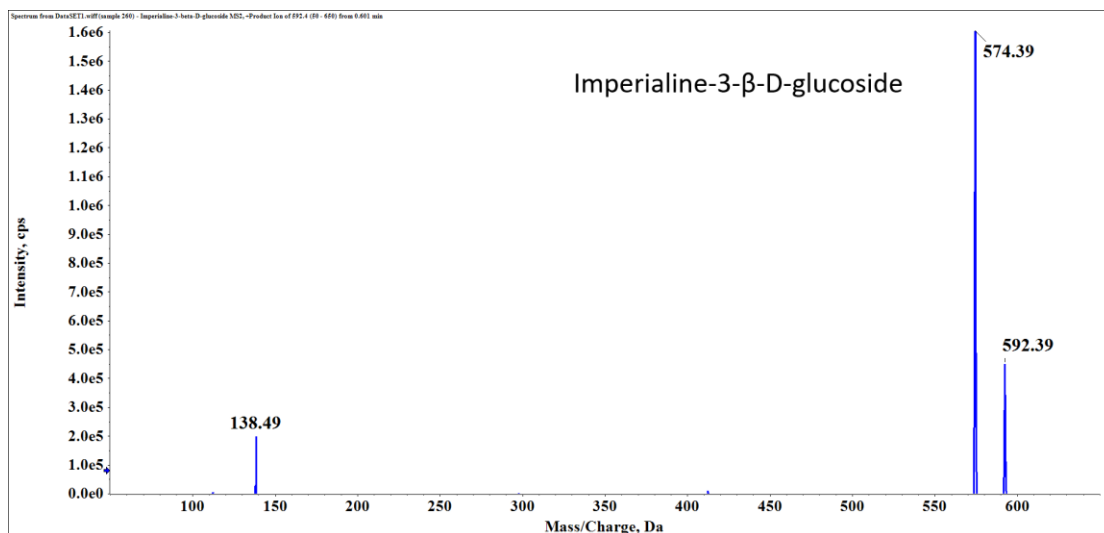
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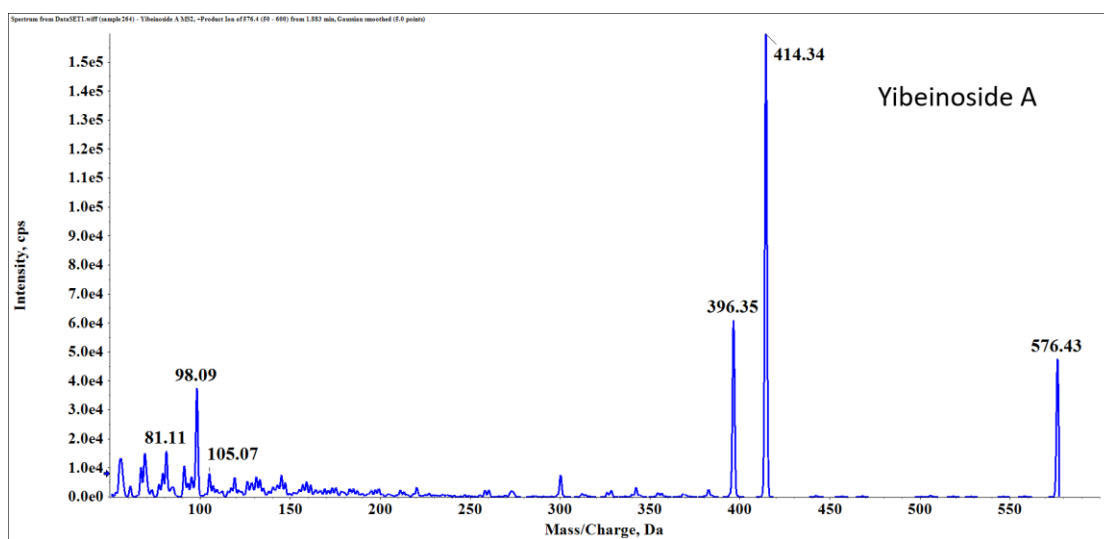
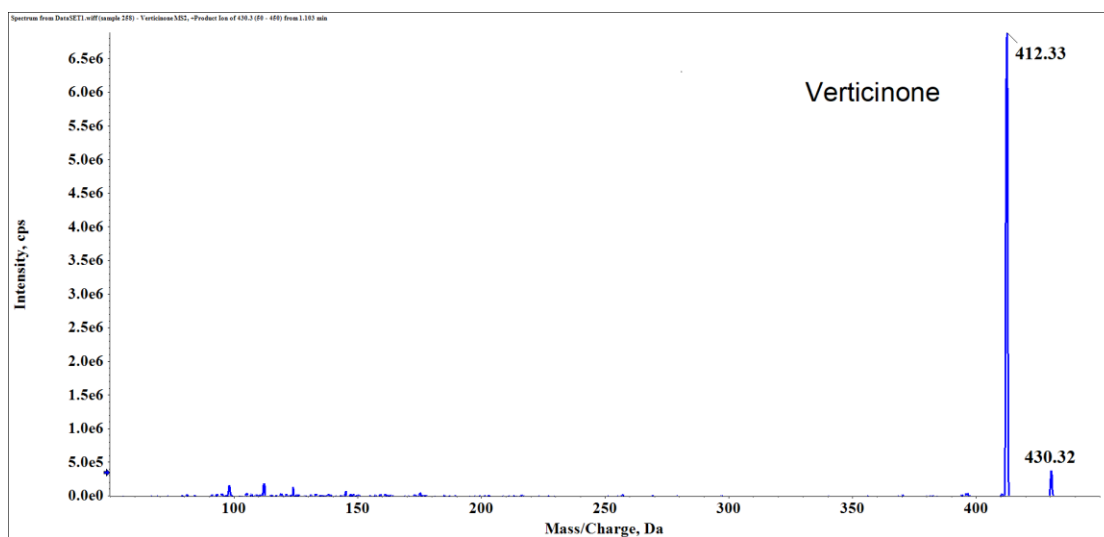
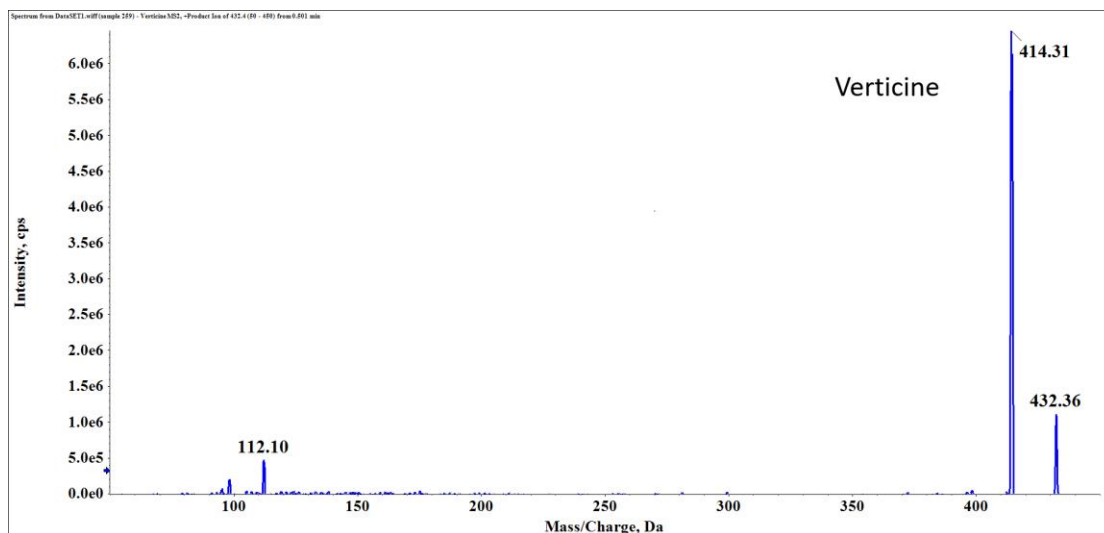
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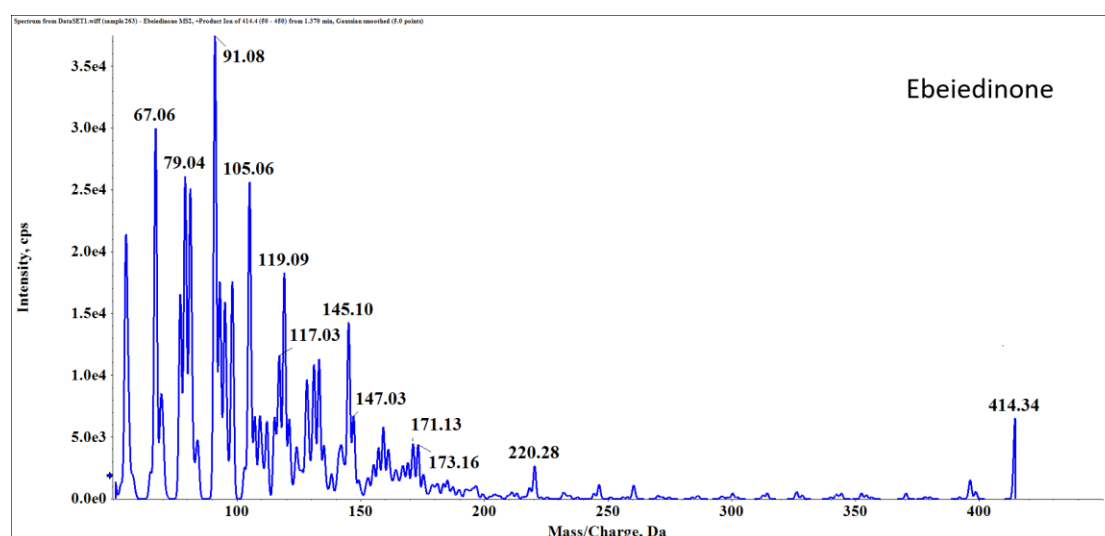
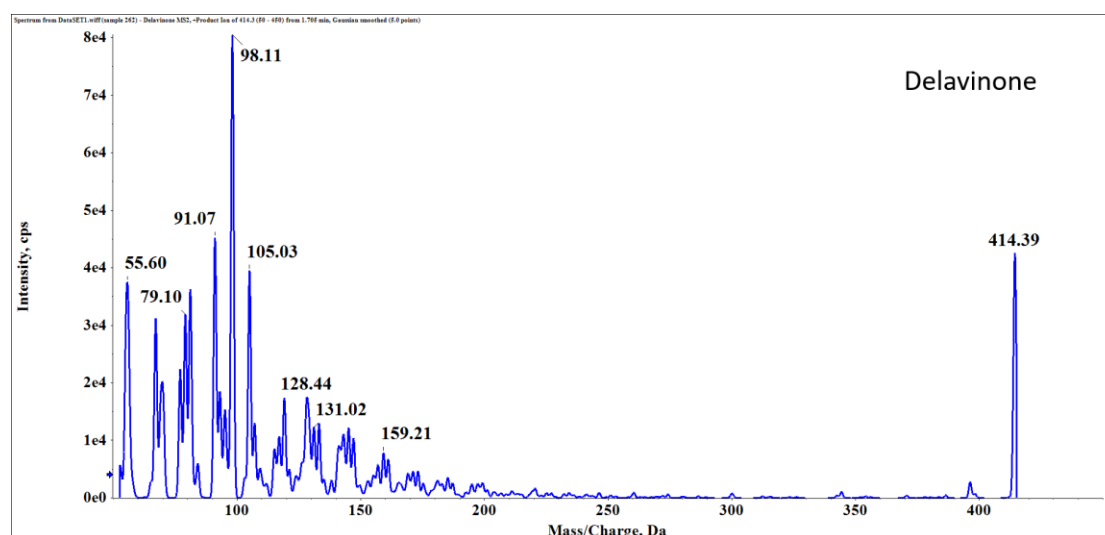
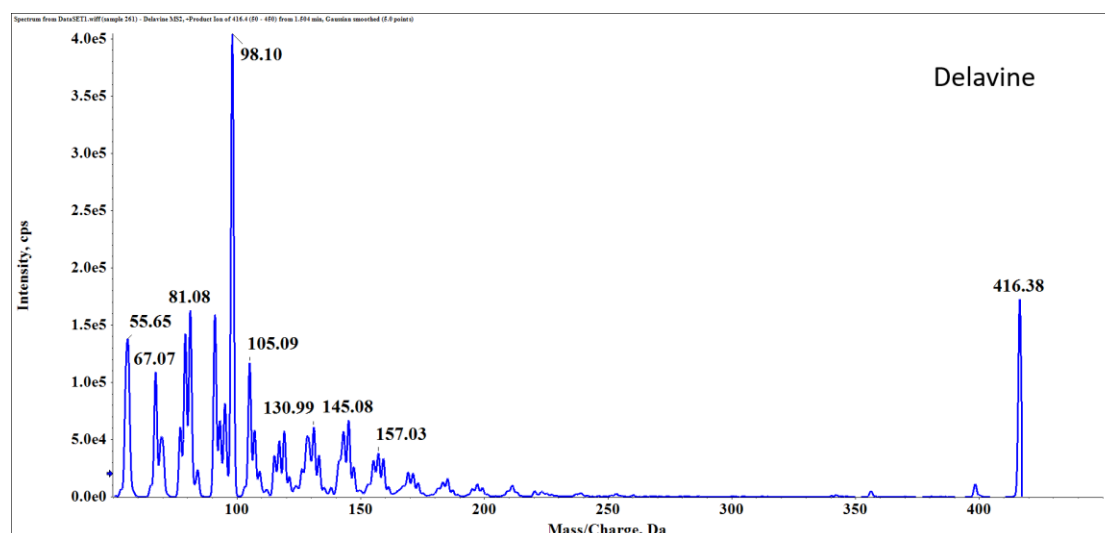


Figure S1. Mass spectrums of nine standard alkaloids

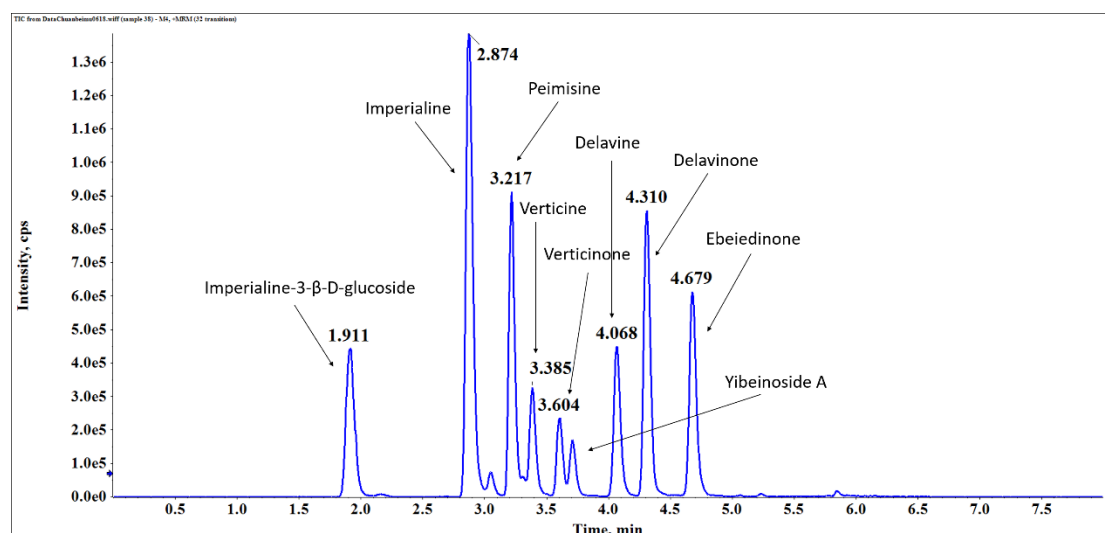


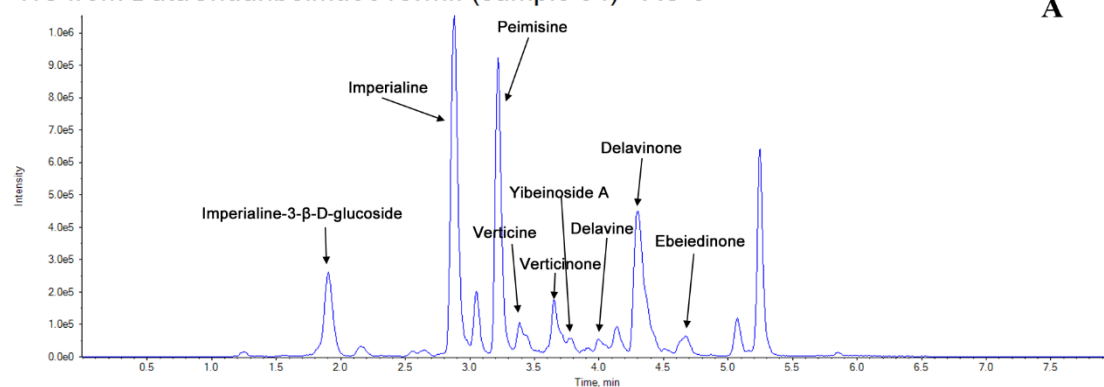
Figure S2. Total ions chromatogram of nine alkaloids in mixed standard solution using the multiple-reaction monitoring (MRM) mode.

Table S1. Linear regression data, linear range, LOD and LOQ, intra- and inter-day precision, repeatability, stability and recovery of nine alkaloids

compounds	Regression	r^2	Linear range	LOD	LOQ	Intra-day	Inter-day	Repeatability	Stability (Standard/Sample)	Average	Recovery
	equation		(ng·mL ⁻¹)	(ng·mL ⁻¹)	(ng·mL ⁻¹)	precision RSD	precision RSD	RSD (%)	RSD (%)	recovery (%)	RSD (%)
						(%)	(%)				
Peimisine	$y=583277x-4637.2$	0.9994	4.883-2500.000	0.2431	0.6173	0.86	1.02	0.92	2.36/1.51	97.42	1.30
Yibeinoside A	$y=123173x-5993.2$	0.9989	4.883-2500.000	0.5426	0.9817	1.04	1.86	1.62	1.87/1.68	96.91	1.11
Ebeiedinone	$y=357471x-381.23$	0.9997	2.441-1250.000	0.1693	0.4025	0.64	1.47	0.65	2.31/1.36	99.33	1.99
Delavinone	$y=452719x-1580.7$	0.9997	4.883-2500.000	0.2704	0.6390	1.27	1.33	1.70	1.26/2.20	100.63	1.49
Delavine	$y=491076x-4806.3$	0.9991	4.883-2500.000	0.3546	0.5752	1.63	1.75	1.94	1.55/1.72	101.22	1.63
Imperialine-3- β -D-glucoside	$y=36376x+45.303$	0.9993	9.766-2500.000	0.2685	0.5487	1.39	2.10	1.03	1.83/1.47	100.13	1.89
Verticine	$y=80297x-1351.1$	0.9975	4.883-2500.000	0.2196	0.6638	0.99	2.39	1.99	1.71/0.91	98.30	1.85
Verticinone	$y=76389x-933.17$	0.9991	2.441-1250.000	0.8273	1.9531	1.58	1.17	1.28	1.64/1.09	101.41	1.59
Imperialine	$y=351515x-5675.2$	0.9992	2.441-1250.000	0.5508	0.8496	0.57	2.26	1.88	1.31/1.93	97.80	1.92

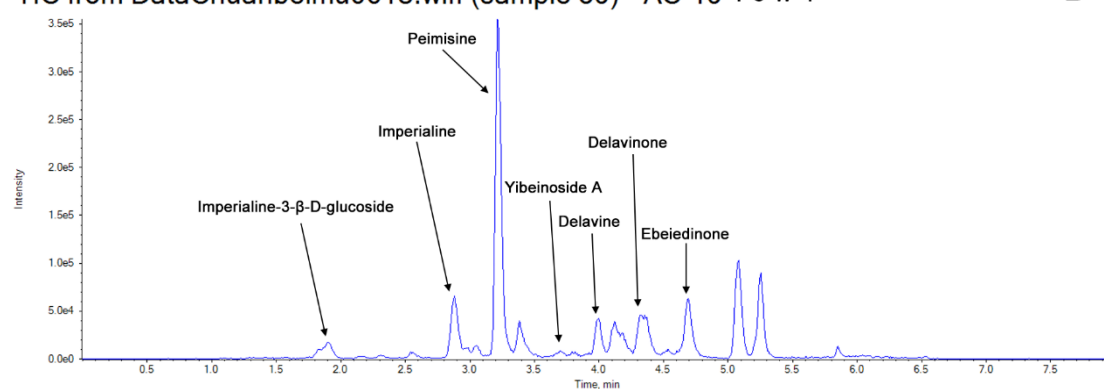
TIC from DataChuanbeimu0618.wiff (sample 54) - AC-3 -Fc-c-4

A



TIC from DataChuanbeimu0618.wiff (sample 59) - AC-19 -Fc-w-1

B



TIC from DataChuanbeimu0618.wiff (sample 83) - BM-22 -Fp-c-7

C

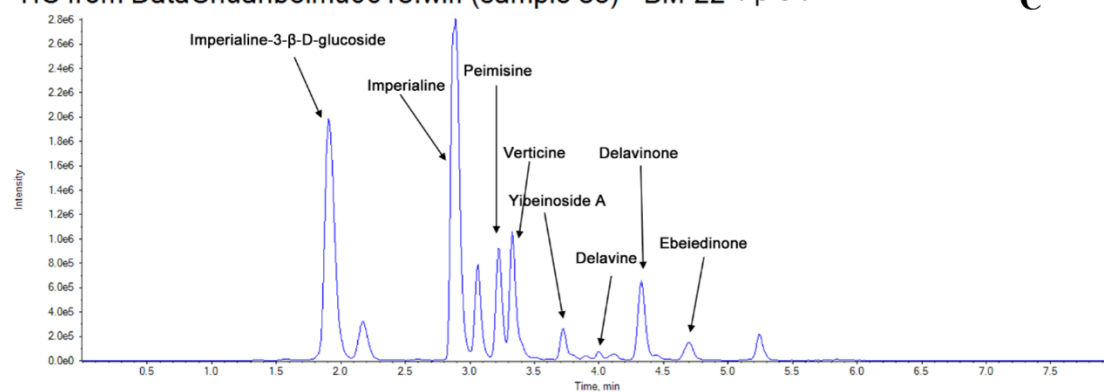


Figure S3. Representative total ions chromatograms of FCB and FPB samples (A: FCB-ZQB.; B: FCB-QB, C: FPB-YB)

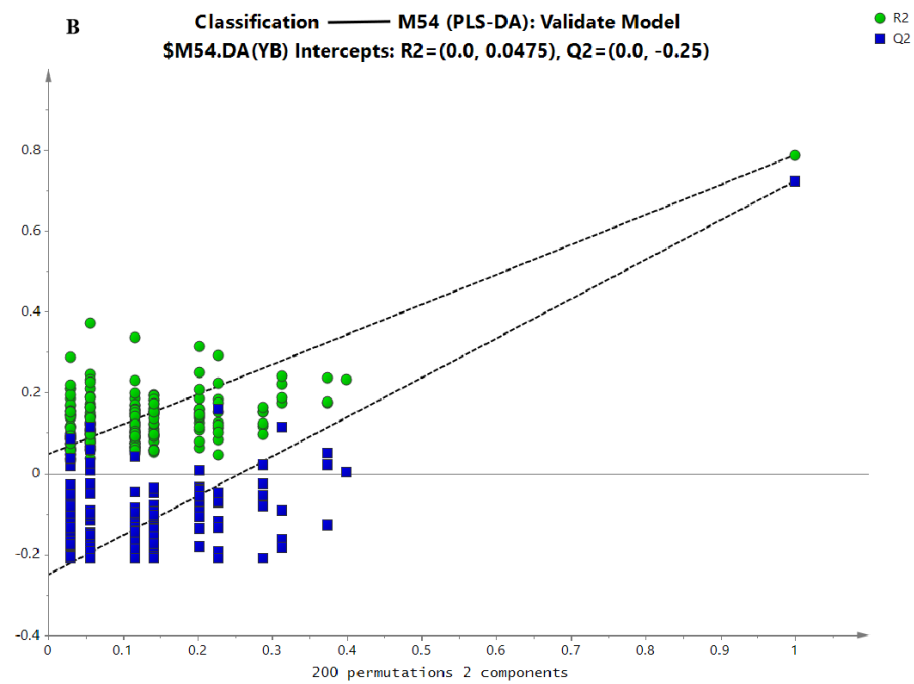
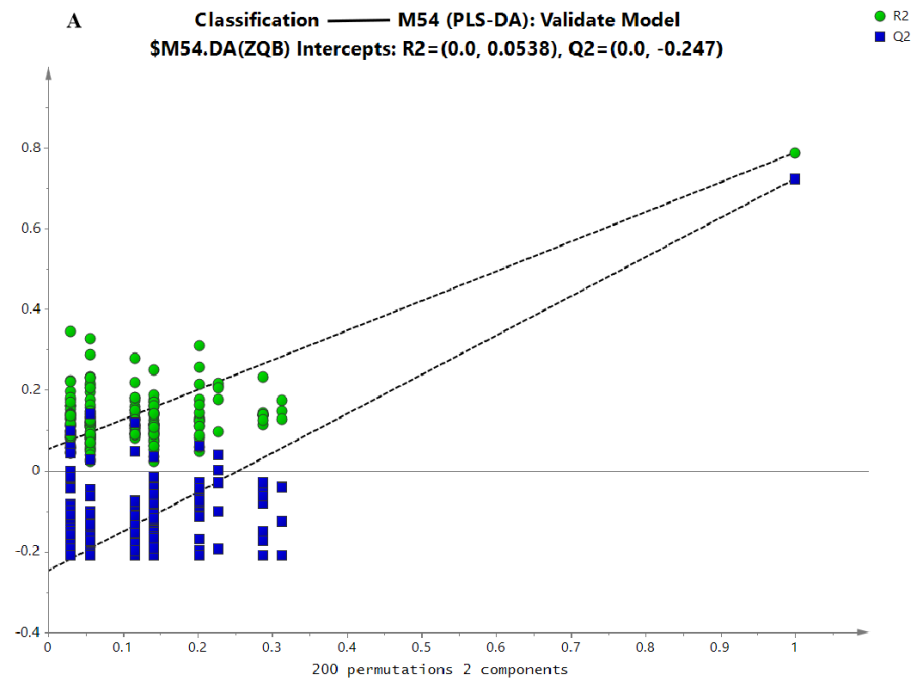
Table S2. The content of nine steroidal alkaloids in FCB and FPB samples

Sample Name	Peimisine	Yibeinoside A	Ebeiedinone	Delavinone	Delavine	Imperialine 3- β -D-glucoside	Verticine	Verticinone	Imperialine
ZQB-1	83.06	7.59	7.48	29.40	1.51	16.52	6.32	4.13	33.58
ZQB-2	81.35	20.64	0.31	71.79	2.52	36.58	1.31	21.36	81.93
ZQB-3	123.53	28.54	10.50	68.94	4.71	68.71	1.69	22.11	72.41
ZQB-4	55.08	11.76	3.11	60.87	14.37	35.65	1.57	17.26	1.09
ZQB-5	113.48	14.09	3.34	43.41	1.25	5.97	3.92	3.43	17.42
ZQB-6	76.35	10.09	6.73	58.85	7.57	19.40	1.47	16.67	50.16
ZQB-7	55.18	7.82	7.45	57.23	2.97	11.82	7.23	5.43	29.97
ZQB-8	74.51	5.68	0.43	42.71	29.18	5.02	6.11	19.58	43.92
ZQB-9	67.03	10.26	16.85	64.12	19.05	27.96	13.06	23.46	56.83
ZQB-10	34.53	12.44	18.88	3.09	4.78	29.69	35.46	35.38	77.07
ZQB-11	25.95	36.16	31.62	46.87	6.09	37.45	59.32	71.36	37.97
ZQB-12	52.26	5.41	13.52	54.18	4.88	3.55	1.21	3.24	23.07
ZQB-13	33.05	4.78	16.38	41.89	13.04	1.74	1.50	4.69	21.10
ZQB-14	24.75	9.13	5.04	9.76	1.37	2.62	5.22	3.65	4.74
ZQB-15	71.26	3.70	22.36	48.30	0.87	3.78	18.93	23.38	23.37
ZQB-16	17.92	3.61	2.38	7.28	0.84	1.54	2.94	7.17	8.85
ZQB-17	28.96	4.14	0.30	29.83	0.76	2.67	1.19	12.61	39.26

ZQB-18	23.30	15.76	58.90	44.54	5.38	15.64	45.11	81.77	8.31
ZQB-19	23.62	6.74	10.91	11.63	6.32	8.05	54.03	34.15	6.59
ZQB-20	69.78	21.99	55.30	26.63	8.63	17.64	46.07	78.13	16.65
ZQB-21	98.01	13.26	11.59	47.97	1.25	18.22	0.00	12.26	40.62
ZQB-22	113.01	17.51	14.82	72.29	2.52	25.83	0.00	17.65	65.75
ZQB-23	108.89	12.07	10.39	66.32	2.58	30.93	0.00	21.55	96.87
ZQB-24	97.67	23.77	6.30	44.05	2.15	55.20	1.34	14.47	57.11
ZQB-25	91.74	22.78	18.44	64.61	2.52	31.13	46.30	41.85	54.65
ZQB-26	103.93	14.22	15.04	57.69	5.59	16.76	22.10	22.79	64.24
ZQB-27	62.01	3.45	4.47	20.27	3.38	7.56	1.11	4.18	37.68
ZQB-28	60.48	19.50	8.59	59.56	5.40	32.39	0.98	10.11	72.41
ZQB-29	167.67	3.08	90.50	1.93	11.40	0.00	27.37	60.23	3.99
ZQB-30	208.26	2.63	107.77	5.02	2.26	0.00	37.98	67.67	3.25
ZQB-31	47.86	4.73	3.61	15.45	1.10	4.72	3.46	5.42	10.01
ZQB-32	55.34	4.63	6.09	18.86	0.95	5.17	3.45	5.77	13.67
ZQB-33	190.56	73.15	54.21	196.53	6.26	619.73	117.34	109.32	680.29
ZQB-34	134.94	51.84	36.06	67.69	4.24	399.66	76.50	123.70	140.23
ZQB-35	111.92	32.36	32.26	61.14	5.54	286.75	57.77	94.14	189.67
ZQB-36	171.00	88.15	21.22	103.03	1.08	474.66	1.47	118.78	255.79
ZQB-37	72.98	8.63	5.78	49.14	1.40	88.35	13.04	38.81	196.16

QB-1	116.3	7.80	10.91	50.66	0.67	0.00	5.52	6.44	5.74
QB-2	49.21	4.80	7.57	37.29	5.52	1.97	2.06	9.43	17.37
QB-3	37.66	2.95	0.68	3.50	0.74	0.00	3.73	2.60	1.59
QB-4	91.88	4.07	19.58	16.90	1.42	2.42	2.99	1.28	2.80
QB-5	47.00	9.14	7.02	44.16	1.81	0.57	5.28	6.17	21.94
QB-6	42.9	7.89	10.21	58.18	0.83	7.03	21.35	23.16	29.27
QB-7	67.85	5.54	12.35	38.70	0.65	1.17	36.33	36.03	10.16
QB-8	90.15	5.30	15.02	56.17	2.21	0.00	2.70	77.87	14.35
QB-9	30.49	3.78	4.60	14.08	1.39	0.00	1.62	2.54	1.57
QB-10	31.36	3.67	11.12	4.23	0.74	0.00	2.45	1.00	3.22
QB-11	88.41	3.02	29.59	5.62	1.04	4.77	1.42	6.44	21.89
QB-12	248.58	4.04	39.83	8.21	2.91	7.49	1.25	2.07	22.27
YB-1	105.35	17.78	54.98	123.44	3.44	61.90	1.57	2.10	246.89
YB-2	49.58	116.49	77.97	158.10	8.25	350.21	1.54	1.98	340.43
YB-3	48.16	38.03	39.77	114.81	5.09	129.20	1.74	1.26	309.26
YB-4	63.37	81.26	82.51	153.40	6.58	288.45	1.35	2.35	332.43
YB-5	28.73	84.43	48.27	50.29	3.34	413.30	1.56	1.37	184.13
YB-6	106.82	382.00	61.94	124.20	7.35	1180.07	2.02	1.83	312.01
YB-7	88.39	209.41	36.46	107.81	7.59	823.50	2.40	1.55	316.98
YB-8	77.37	98.37	86.68	148.37	7.47	316.20	12.86	7.61	344.09

YB-9	62.69	86.72	52.73	127.42	6.51	323.61	1.59	1.78	293.44
YB-10	26.09	63.68	43.24	57.09	2.89	259.65	1.97	1.61	183.82
YB-11	37.63	63.10	33.14	71.93	5.17	332.64	1.38	1.48	247.69
YB-12	54.72	46.15	29.52	92.76	4.40	1.38	1.83	41.18	243.97
YB-13	65.90	82.62	68.55	82.76	1.94	577.56	1.25	1.32	248.61
YB-14	216.05	144.76	55.89	279.53	27.11	61.69	0.00	0.00	78.05
YB-15	100.98	55.42	27.77	121.90	6.82	1.02	1.92	0.00	111.40
YB-16	58.89	112.31	30.71	71.09	3.72	1.51	1.65	1.29	226.88
YB-17	234.59	95.20	41.21	231.47	27.35	73.56	1.32	1.23	149.66



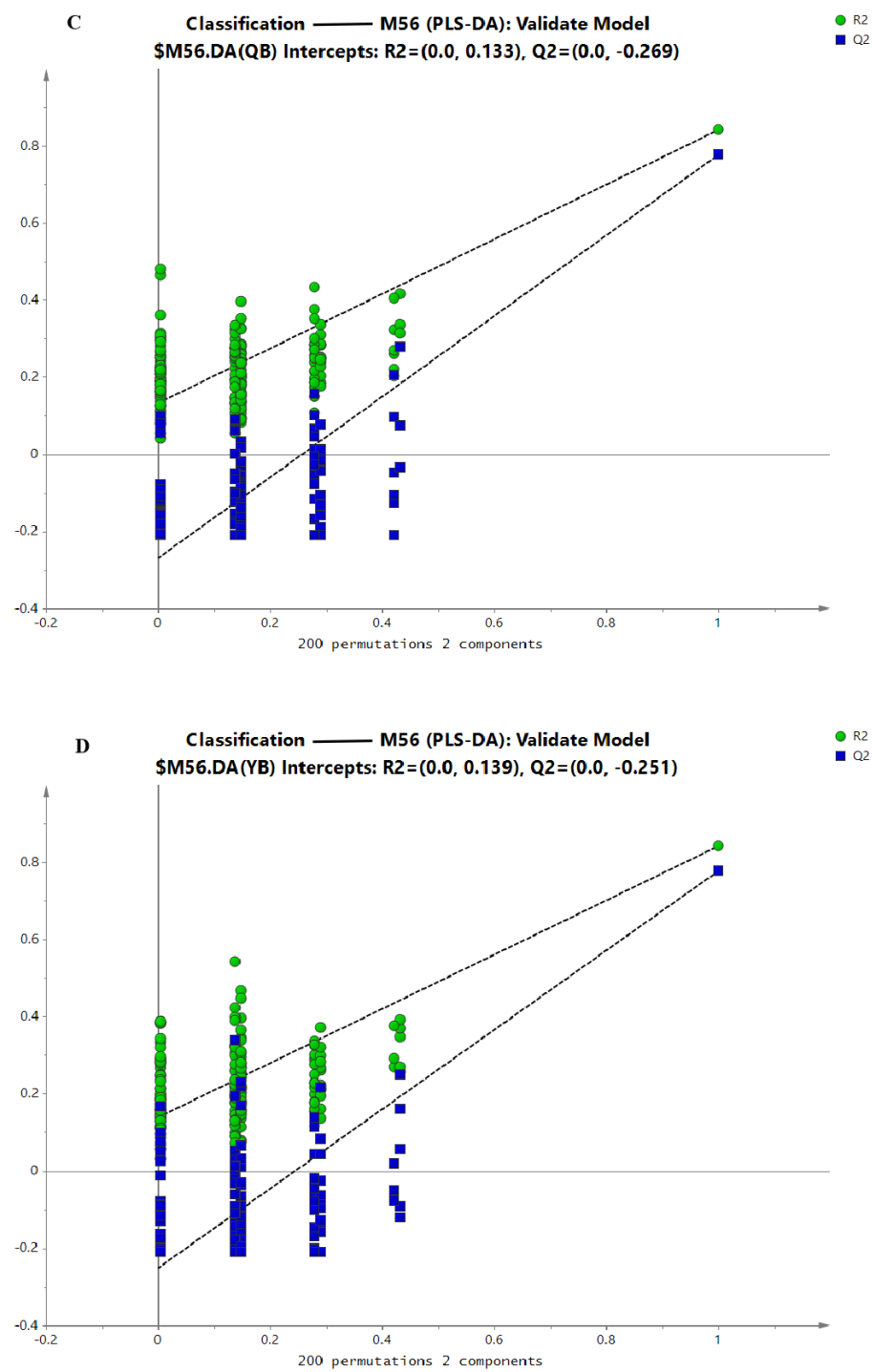


Figure S4. The permutation plot of the PLS-DA models (A,B: validate model for Fig. 5B; C,D: validate model for Fig. 5D)