

Supplementary data

**Real-time monitoring of the column chromatographic process of
Phellodendri Chinensis Cortex Part I: End-point determination based
on near-infrared spectroscopy combined with machine learning**

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Table S1 Results of the raw data using different preprocessing method

Pretreatment method	Berberine hydrochloride		Phellodendrine chloride		Total alkaloids	
	PCs	RMSECV (mg/mL)	PCs	RMSECV (mg/mL)	PCs	RMSECV (mg/mL)
Raw spectra	13	0.0788	11	0.2439	12	0.0767
MSC	11	0.0779	13	0.2385	11	0.0672
SNV	11	0.0752	12	0.2351	13	0.0557
1 st derivative	13	0.1588	9	0.2837	7	0.1975
2 nd derivative	4	0.2166	3	0.3299	4	0.2364
Savitzky–Golay	10	0.0976	8	0.2755	11	0.0739
SNV+ Savitzky–Golay	13	0.0670	10	0.2457	12	0.0546
1 st derivative + Savitzky–Golay	11	0.1510	9	0.2791	7	0.1954
SNV+1 st derivative	7	0.1706	8	0.2695	14	0.1407

Table S2 Results of the selected variables data by SPA using different preprocessing methods

Pretreatment method	Berberine hydrochloride		Phellodendrine chloride		Total alkaloids	
	PCs	RMSECV (mg/mL)	PCs	RMSECV (mg/mL)	PCs	RMSECV (mg/mL)
Raw spectra	13	0.1091	7	0.3455	11	0.1211
MSC	10	0.1098	5	0.3030	9	0.1211
SNV	10	0.1145	6	0.3013	12	0.1204
1 st derivative	12	0.1342	3	0.4256	12	0.1569
2 nd derivative	10	0.1372	3	0.3733	10	0.1679
Savitzky–Golay	8	0.1590	3	0.4164	9	0.1705
SNV+ Savitzky–Golay	10	0.1455	3	0.3282	11	0.1904
1 st derivative + Savitzky–Golay	7	0.1656	2	0.4082	10	0.1731
SNV+1 st derivative	12	0.1344	3	0.3593	7	0.1812

Table S3 Results of selected variables data by UVE after different pretreatment methods for the target compounds

Pretreatment method	Berberine hydrochloride		Phellodendrine chloride		Total alkaloids	
	PCs	RMSECV (mg/mL)	PCs	RMSECV (mg/mL)	PCs	RMSECV (mg/mL)
Raw spectra	13	0.1409	8	0.2892	10	0.1379
MSC	8	0.1335	8	0.2862	9	0.1461
SNV	9	0.1344	7	0.2930	9	0.1183
1 st derivative	10	0.1380	6	0.2967	10	0.1488
2 nd derivative	13	0.1478	9	0.3015	12	0.1770
Savitzky–Golay	12	0.1528	9	0.2887	9	0.1497
SNV+ Savitzky–Golay	11	0.1573	8	0.2905	10	0.1240
1 st derivative + Savitzky–Golay	13	0.1536	11	0.3119	9	0.1662
SNV+1 st derivative	14	0.1500	9	0.2928	11	0.1227

Table S4 Results of selected variables data by CARS after different pretreatment methods for the target compounds

Pretreatment method	Berberine hydrochloride		Phellodendrine chloride		Total alkaloids	
	PCs	RMSECV (mg/mL)	PCs	RMSECV (mg/mL)	PCs	RMSECV (mg/mL)
Raw spectra	11	0.0614	10	0.3053	11	0.0520
MSC	8	0.0676	7	0.2817	10	0.0528
SNV	9	0.0650	8	0.2791	11	0.0498
1 st derivative	11	0.0793	5	0.3429	14	0.0702
2 nd derivative	10	0.1324	4	0.3458	12	0.1087
Savitzky–Golay	11	0.0914	5	0.3004	13	0.0625
SNV+ Savitzky–Golay	11	0.0655	4	0.3006	13	0.0522
1 st derivative + Savitzky–Golay	10	0.0715	5	0.3094	10	0.0769
SNV+1 st derivative	13	0.0714	4	0.3079	9	0.0899