Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

A comprehensive strategy to monitor quality consistency of Weibizhi tablets based on integrated MIR and UV spectroscopic fingerprints, a systematically quantified fingerprint method, antioxidant activities and UPLC–Q-TOF-MS chemical profiling

Contents

Table S1. Constituents in WBZT identified by UPLC–Q-TOF-MS in positive ion mode.

No.	t_R (min)	Identification	Positive ion (*m/z*)		Elemental composition	Molecular weight (Da)	MS/MS (*m/z*)	Source
			Measured mass	ppm				
1	3.77	liquiritin apioside	551.1754	- 2.0	$C_{26}H_{30}O_{13}$	550.1686	551; 419; 257; 147; 137; 119	licorice
2	3.92	liquiritin	419.1345	- 2.1	$C_{21}H_{22}O_9$	418.1264	419; 257; 137; 119	licorice
3	4.73	isoliquiritin apioside	551.1753	- 2.2	$C_{26}H_{30}O_{13}$	550.1686	551; 419; 257; 147; 137; 119	licorice
4	5.13	isoliquiritin	419.1341	- 0.24	$C_{21}H_{22}O_9$	418.1186	419; 257; 145; 137; 119	licorice
5	5.34	neoisoliquiritin	419.1337	- 1.2	$C_{21}H_{22}O_9$	418.1186	419; 255; 147; 137; 119	licorice
6	5.40	ononin	431.1339	- 0.70	$C_{22}H_{22}O_9$	430.1264	431; 269; 255; 137; 145	licorice
7	6.21	liquiritigenin	257.0816	- 0.78	$C_{15}H_{12}O_4$	256.0736	257; 147; 137; 119	licorice
8	8.53	licorice-saponin G_2	839.4044	- 2.5	$C_{42}H_{62}O_{17}$	838.3987	839; 487; 469	licorice
9	9.03	isoliquiritigenin	257.0814	0.2	$C_{15}H_{12}O_4$	256.0736	257; 147; 137; 119	licorice
10	9.40	glycyrrhizic acid	823.4111	- 0.61	$C_{42}H_{62}O_{16}$	822.4038	823; 647; 413; 453	licorice
11	10.34	licorice-saponin H_2	823.4104	- 1.5	$C_{42}H_{62}O_{16}$	822.4038	823; 471; 453	licorice
12	10.66	licorice-saponin K_2	823.4106	- 2.4	$C_{42}H_{62}O_{16}$	822.4038	823; 453	licorice
13	11.18	inflacoumarin A	323.1290	2.2	$C_{20}H_{18}O_4$	322.1205	323; 267; 239; 121	licorice
14	11.78	licorice-saponin B_2	809.4311	- 1.6	$C_{42}H_{64}O_{15}$	808.4245	809; 439	licorice
15	13.12	18-α-glycyrrhetinic acid 3-O-glucuronide	647.3797	- 0.31	$C_{36}H_{54}O_{10}$	646.3717	647; 453	licorice
16	13.68	licochalcone A	339.1599	- 0.88	$C_{21}H_{22}O_4$	338.1518	339; 271; 121	licorice
17	14.39	18-β-glycyrrhetinic acid 3-O-glucuronid	647.3779	- 0.89	$C_{36}H_{54}O_{10}$	646.3717	647; 453	licorice
18	16.18	licoflavone A	393.2061	- 1.3	$C_{25}H_{28}O_4$	392.1988	393; 337; 203; 149	licorice
19	18.27	18-α-glycyrrhetinic acid	471.3472	- 0.42	$C_{30}H_{46}O_4$	470.3396	471; 453; 317	licorice
20	18.46	18-β-glycyrrhetinic acid	471.3470	- 0.85	$C_{30}H_{46}O_4$	470.3396	471; 453; 317	licorice

Table S2. **The measured and predicted EC_{50} values of 27 WBZT samples.**

Sample No.	Measured EC_{50} (mg/mL, mean ± SD, n = 3)	Measured EC_{50} (mg/mL)	Predicted EC_{50} (mg/mL)	RE[c] (%)
S1[b]	0.694±0.007	0.694	0.714	0.029
S2[a]	0.641±0.006	0.641	0.637	–0.006
S3[a]	0.585±0.005	0.585	0.557	–0.048
S4[b]	0.661±0.008	0.661	0.682	0.031
S5[a]	0.661±0.007	0.661	0.666	0.008
S6[a]	0.771±0.009	0.771	0.742	–0.037
S7[a]	0.679±0.008	0.679	0.706	0.039
S8[a]	0.712±0.009	0.712	0.718	0.008
S9[a]	0.684±0.006	0.684	0.694	0.015
S10[a]	0.649±0.003	0.649	0.657	0.012
S11[a]	0.736±0.006	0.736	0.717	–0.026
S12[a]	0.721±0.007	0.721	0.718	–0.004
S13[a]	0.663±0.006	0.663	0.671	0.012
S14[a]	0.663±0.008	0.663	0.683	0.030
S15[a]	0.630±0.007	0.630	0.631	0.002
S16[a]	0.729±0.008	0.729	0.722	–0.010
S17[d]	0.446±0.002	0.76	–	–
S18[b]	0.632±0.006	0.632	0.634	0.003
S19[a]	0.753±0.010	0.753	0.741	–0.016
S20[b]	0.657±0.007	0.657	0.666	0.014
S21[a]	0.595±0.006	0.595	0.612	0.029
S22[b]	0.712±0.011	0.712	0.704	–0.011
S23[a]	0.826±0.012	0.826	0.814	–0.015
S24[a]	0.694±0.007	0.694	0.717	0.033
S25[d]	0.522±0.005	0.89	–	–
S26[a]	0.602±0.003	0.602	0.591	–0.018
S27[b]	0.585±0.005	0.585	0.612	0.046

a) Calibration sets; b) Validation sets; c) RE, relative error; d) Identified outliers.

Fig. S1. Score plot of principal components t[1] versus t[2] used to find outliers for PLSR analysis. The ellipse corresponds to the confidence intervals based on HotellingT^2 (0.05).