Electronic Supplementary Material (ESI) for Analytical Methods.

A Modified QuEChERS Method Coupled with High Resolution LC-Q-TOF-Mass Spectrometry for Extraction, Identification and Quantification of Isoflavones in the Soybeans

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SUPPORTING INFORMATION

Fig. S1 Extracted ion chromatograms of six authentic isoflavone compounds

Fig. S2 IDA-MS spectrum of six authentic isofalvones

Fig. S3 The trend chart of range value for daidzin concentration

Fig. S4 The trend chart of range value for daidzein concentration

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Equations. The equations of RSM design

Fig. S1 Extracted ion chromatograms of six authentic isoflavone compounds

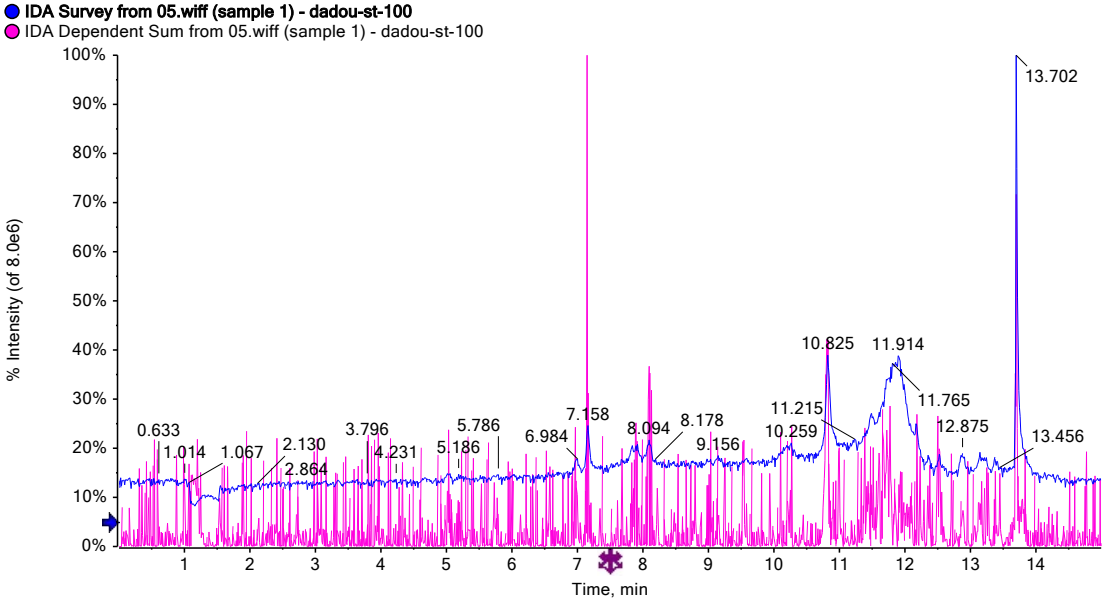
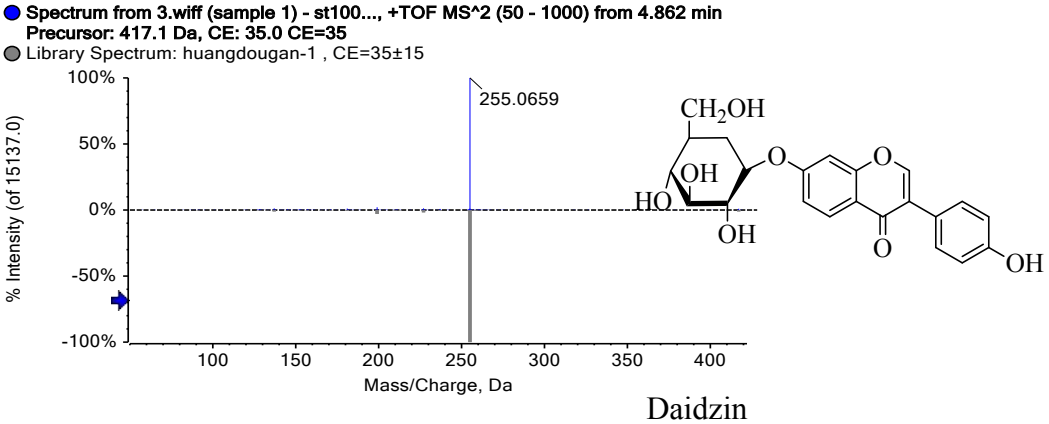
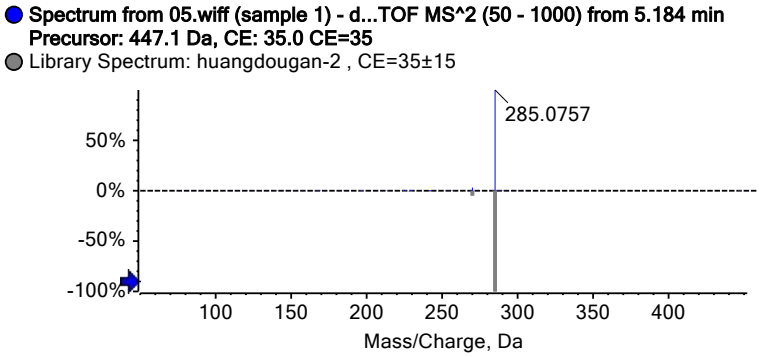
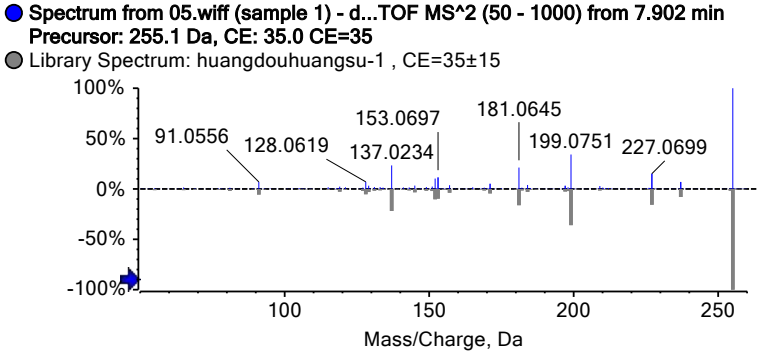


Fig. S2 IDA-MS spectrum of six authentic isofalvones

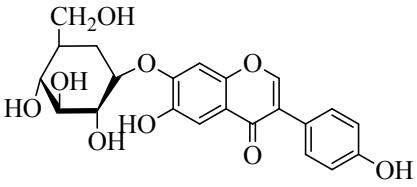


Daidzin

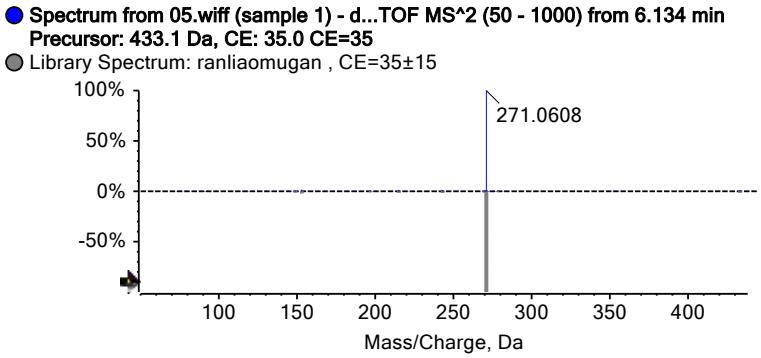


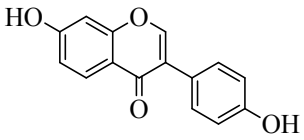


Glycitin

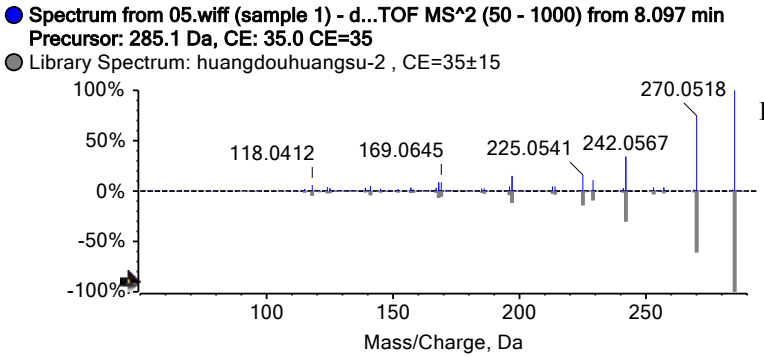


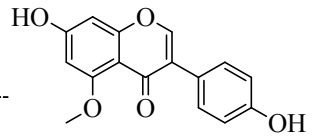
Genistin



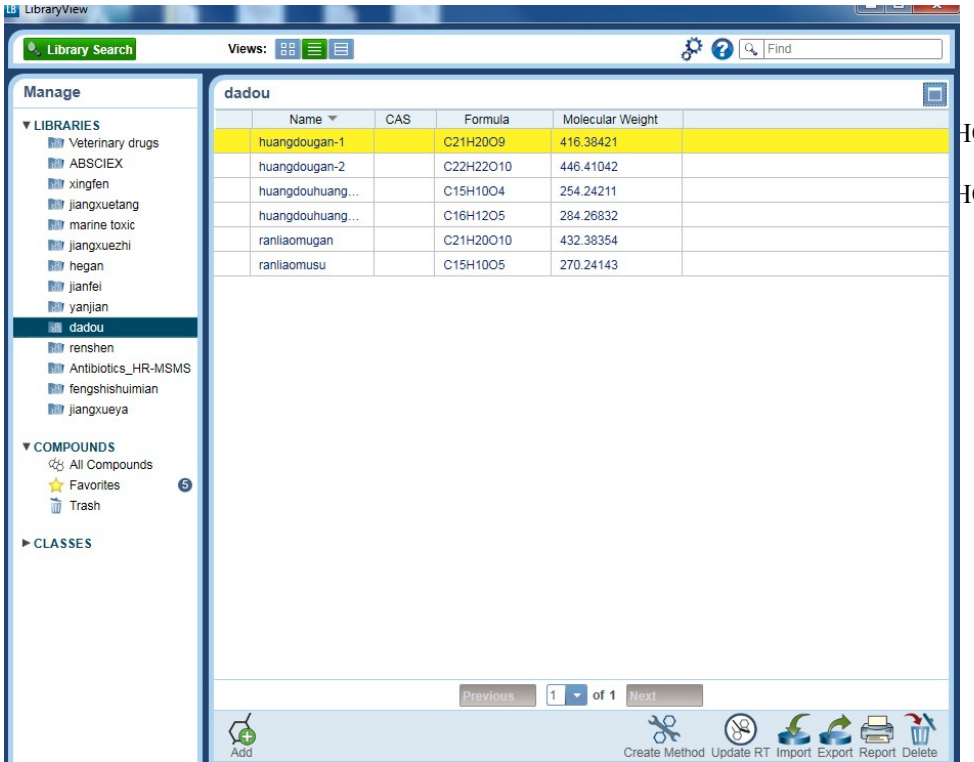


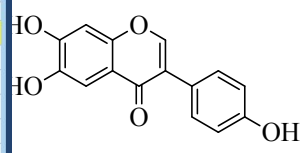
Daidzein





Glycitein





Genistein

Fig. S3 The trend chart of range value for daidzin concentration

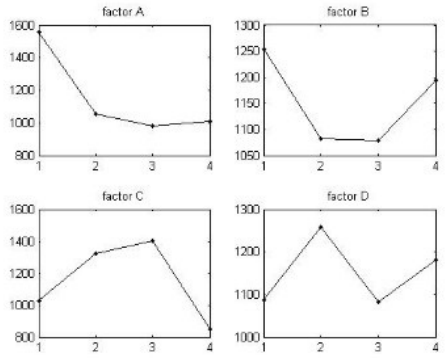


Fig. S4 The trend chart of range value for daidzein concentration

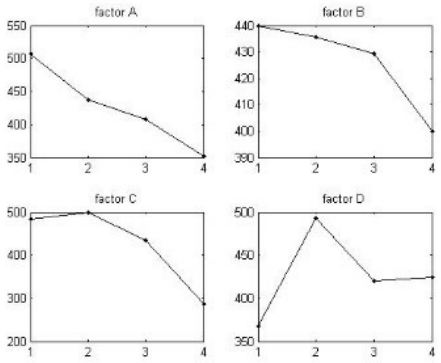


Table S1 The Quantitative Analysis of Mass data for isoflavones

Peak No.	Compounds	Formula	Ions	Theoretical(m/z)	Experimental (m/z)	Error(ppm)	retention time(min)
1	Daidzin	$C_{21}H_{20}O_9$	$[M+H]^+$	417.11801	417.11830	0.7	6.20
2	Glycitin	$C_{22}H_{22}O_{10}$	$[M+H]^+$	447.12857	447.12892	0.8	6.35
3	Genistin	$C_{21}H_{20}O_{10}$	$[M+H]^+$	433.11292	433.11296	0.1	7.32
4	Daidzein	$C_{15}H_{10}O_4$	$[M+H]^+$	255.06519	255.06540	0.9	8.68
5	Glycitein	$C_{16}H_{12}O_5$	$[M+H]^+$	285.07575	285.07601	0.9	8.82
6	Genistein	$C_{15}H_{10}O_5$	$[M+H]^+$	271.06010	271.06018	0.3	9.73

Table S2 The results of analysis of range for daidzin concentration

T value: 1.0e+003*					
	1.5588	1.2544	1.0280	1.0870	1.1460
	1.0557	1.0818	1.3237	1.2582	1.1887
	0.9843	1.0780	1.4054	1.0823	1.2027
	1.0090	1.1934	0.8507	1.1803	1.0703
R value :		574.48	176.41	554.67	175.96
		132.37			
optimal level :		1 1 3 2 3			
order:		A; C; B; D			

Table S3 The Results of Analysis of Variance for Daidzin

sources of variance	sum of squares	freedom	Standard deviation	F value	F^{α}	significance
factor 1	5.5830e+004	3	1.8610e+004	14.0456	4.7571;9.7795	high significance
factor 2	5.6509e+003	3	1.8836e+003	1.4217	4.7571;9.7795	
factor 3	4.9957e+004	3	1.6652e+004	12.5681	4.7571;9.7795	high significance
factor 4	5.2940e+003	3	1.7647e+003	1.3318	4.7571;9.7795	
blank list*	2.6559e+003	3	885.2891	0.6682	4.7571;9.7795	
error	7.9498e+003	6	1.3250e+003			
sum	1.1939e+005	15				

Table S4 The results of analysis of range for daidzein concentration

T value:					
	506.75	439.70	483.54	367.88	405.04
	437.68	435.73	498.13	492.80	453.74
	407.91	429.17	435.32	419.87	423.40
	352.17	399.91	287.52	423.96	422.33
R value :		154.58	39.79	210.61	124.92
		48.70			
optimal level :		1 1 2 2 2			
order:		C; A; D; B			

Table S5 The Results of Analysis of Variance for Daidzein

sources of variance	sum of squares	freedom	Standard deviation	F value	F^{α}	significance
factor 1	3.1088e+004	3	1.0363e+003	11.2942	4.7571;9.7795	high significance
factor 2	243.2587	3	81.0862	0.8838	4.7571;9.7795	
factor 3	6.9443e+003	3	2.3148e+003	25.2287	4.7571;9.7795	high significance
factor 4	1.9705e+003	3	653.8207	7.1587	4.7571;9.7795	significance
blank list*	307.2483	3	102.4161	1.1162	4.7571;9.7795	
error	550.5070	6	91.7512			
sum	1.2574e+004	15				

Table S6 Analysis of Variance for the Fitted Quadratic Polynomial Model on Daidzin

sources	sum of squares	df	mean square	F value	p-value prob>F	significant
Model	28320.60	9	3146.73	1.20	0.4163	not significant
X1	3112.05	1	312.05	1.18	0.3130	
X2	270.61	1	270.61	0.10	0.7579	
X3	2709.00	1	2709.00	1.03	0.3442	
X1X2	7745.32	1	7745.32	2.94	0.1300	
X1X3	4003.28	1	4003.28	1.52	0.2573	
X2X3	6371.63	1	6371.63	2.42	0.1637	
X12	34.95	1	34.95	0.013	0.9115	
X22	2616.61	1	2616.61	0.99	0.3520	
X32	1181.57	1	1181.57	0.45	0.5244	
Residual	18429.78	7	2632.83			
Lack of fit	11838.31	3	3946.10	2.39	0.2090	not significant
Pure error	6591.47	4	1647.87			
Cor Total	46750.37	16				

Table S7 Analysis of Variance for the Fitted Quadratic Polynomial Model on Daidzein

sources	sum of squares	df	mean square	F value	p-value prob>F	significant
Model	1213.14	9	134.79	1.38	0.3414	not significant
X1	76.57	1	76.57	0.79	0.4046	
X2	221.66	1	221.66	2.28	0.1750	
X3	6.82	1	6.82	0.070	0.7989	
X1X2	162.22	1	162.22	1.67	0.2377	
X1X3	620.58	1	620.58	6.38	0.0395	
X2X3	14.41	1	14.41	0.15	0.7119	
X12	97.78	1	97.78	1.00	0.3496	
X22	8.16	1	8.16	0.084	0.7806	
X32	0.34	1	0.34	3.489E-003	0.9545	
Residual	681.39	7	97.34			
Lack of fit	449.40	3	149.80	2.58	0.1908	not significant
Pure error	231.99	4	58.00			
Cor Total	1894.53	16				

Equations. The equations of RSM design

Equation 1:

$$x_i = (X_i - X_0) = \Delta X \quad (1)$$

Where x_i was the value of the independent variable X_i ,X_0 was the value of X_i at the center point, and ΔX was the step change value.

Equation 2:

$$Y = b_0 + \sum_{i=1}^{3} A_i X_i + \sum_{i=1}^{3} A_{ii} X_i^2 + \sum_{i=1}^{2} \sum_{j=i+1}^{3} A_{ij} X_i X_j \quad (2)$$

Where Y was the predicted variable function and A_i, A_{ii}, and A_{ij} were the regression coefficient of linear, quadratic, and interaction terms of independent variables X_i and X_j.

Equation 3:

$$y_{daidzin} = 207.56 + 19.72X_1 + 5.82X_2 + 18.40X_3 - 44.00X_1X_2 - 31.64X_1X_3 + 39.91X_2X_3 + 2.88X \quad (3)$$

Equation 4:

$$y_{daidzein} = 89.35 + 3.09X_1 + 5.26X_2 + 0.92X_3 - 6.37X_1X_2 - 12.46X_1X_3 + 1.90X_2X_3 + 4.82X_1^2 + 1.3$$