Supplementary Materials

Table S1. The ANOVA for special quartic mixture model.

Sourse	R1		R2		R3		R4		R5		R6	
	F	P	F	P	F	P	F	P	F	P	F	P
Model	26.71	0.0001 ^{S}	64.80	< 0.0001 ^{S}	32.88	< 0.0001 ^{S}	127.38	< 0.0001 ^{S}	19.42	0.0004 ^{S}	110.89	< 0.0001 ^{S}
Linear	85.49	< 0.0001 ^{S}	132.57	< 0.0001 ^{S}	103.77	< 0.0001 ^{S}	465.31	< 0.0001 ^{S}	9.58	0.0099 ^{S}	203.52	< 0.0001 ^{S}
AB	10.11	0.0155 ^{S}	10.37	0.0146 ^{S}	18.75	0.0034 ^{S}	19.02	0.0033 ^{S}	7.12	0.0321 ^{S}	61.23	0.0001 ^{S}
AC	4.94	0.0617 ^{NS}	23.25	0.0019 ^{S}	13.78	0.0075 ^{S}	24.05	0.0017 ^{S}	53.01	0.0002 ^{S}	427.64	< 0.0001 ^{S}
BC	10.49	0.0143 ^{S}	12.24	0.0100 ^{S}	19.22	0.0032 ^{S}	19.37	0.0032 ^{S}	9.28	0.0187 ^{S}	66.07	< 0.0001 ^{S}
A^2BC	3.46	0.1052 ^{NS}	26.88	0.0013 ^{S}	13.44	0.0080 ^{S}	4.15	0.0810 ^{NS}	18.75	0.0034 ^{S}	90.34	< 0.0001 ^{S}
AB^2C	6.36	0.0397 ^{S}	0.091	0.7714 ^{NS}	3.24	0.1149 ^{NS}	5.71	0.0482 ^{S}	1.57	0.2506 ^{NS}	24.71	0.0016 ^{S}
ABC^2	6.90	0.0341 ^{S}	13.84	0.0074 ^{S}	4.09	0.0829 ^{NS}	3.23	0.1155 ^{NS}	0.027	0.8733 ^{NS}	43.90	0.0003 ^{S}
LOF	19.85	0.0042 ^{S}	16.48	0.0063 ^{S}	155.37	< 0.0001 ^{S}	21.97	0.0033 ^{S}	24.58	0.0026 ^{S}	6.96	0.0359 ^{S}

F: Test statistic, P: *p*-value, LOF: Lack of Fit.

^{S} means significant, ^{NS} means not significant.

Table S2. The results of complete or reduced special-quartic mixture models fit to six responses.

Model term in pseudo-components	Model coefficients estimated from data [a]					
	R1	R2	R3	R4	R5	R6
z_1	4.01	2.04	11.22	1.55	9.10	6.12
z_2	52.02	64.47	243.64	85.80	101.07	90.77
z_3^2	4.37	2.79	12.76	2.56	9.67	6.03
z_1z_2	-51.90	-67.49	-264.59	-93.86	-97.81	-93.60
z_1z_3	0.35	-0.98	-2.21	1.03	-2.60	-2.41
z_2z_3	-53.03	-73.53	-268.68	-95.02	-112.02	-97.53
$z_1^2z_2z_3$	24.31	-87.00	179.39	35.11	127.13	91.04
$z_1z_2^2z_3$	-291.61	44.83	-779.22	-364.42	-325.30	-421.24
$z_1z_2z_3^2$	36.62	66.60	105.52	33.03	-5.18	67.70
Summary statistics						
R-Squared	0.9683	0.9368	0.9741	0.9932	0.9569	0.9922
Adj R-Squared	0.9320	0.9714	0.9444	0.9854	0.9076	0.9832
Pred R-Squared	0.8561	0.9368	0.8680	0.9156	0.8882	0.8997

[a] Coefficient was statistically significant with at least 95% confidence.

Table S3. The constraints and results of numerical optimization with desirability function.

Parameter	Goal	Experimental region		Weight		Importance	Solutions				
		Lower	Upper	Lower	Upper		1	2	3	4	5
Water	In range	93.5	97.9	1	1	3	**93.9**	95.568	95.7	97.171	97.513
Oil	In range	0.1	0.5	1	1	3	**0.1**	0.5	0.3	0.5	0.1
Surfctant	In range	2	6	1	1	3	**6**	3.932	4	2.329	2.387
R1	Maxmize	3.98	4.40	1	1	5	**4.36**	4.29	4.32	4.11	4.07
R2	Maxmize	1.50	2.67	1	1	5	**2.64**	1.88	1.83	1.73	2.03
R3	Maxmize	10.42	12.49	1	1	5	**12.44**	11.66	11.47	10.92	11.18
R4	Maxmize	1.24	2.56	1	1	5	**2.55**	2.02	2.14	1.57	1.72
R5	Maxmize	8.70	9.45	1	1	5	**9.40**	9.05	8.89	9.59	8.94
R6	Maxmize	5.47	6.12	1	1	5	**5.84**	6.03	5.83	6.14	5.92
Desirability							**0.876**	0.568	0.471	0.39	0.374

Table S4. Q-TOF MS accurate measurements for the six analytes.

No.	Proposal ion	Experimental *m/z*	Theoretical *m/z*	Diff (ppm)	Elemental composition
1	$[M-H]^-$	353.0888	353.0878	-2.81	$C_{16}H_{18}O_9$
	[M-H-caffeoyl] $^-$	191.0559	191.0561	1.10	$C_7H_{12}O_6$
2	$[M-H]^-$	447.0925	447.0933	1.75	$C_{21}H_{20}O_{11}$
	$[M-H-Glc]^-$	285.0392	285.0405	4.41	$C_{15}H_{10}O_6$
3	$[M-H]^-$	515.1209	515.1195	-2.71	$C_{25}H_{24}O_{12}$
	[M-H-caffeoyl] $^-$	353.0876	353.0878	0.58	$C_{16}H_{18}O_9$
	[M-H-2caffeoyl] $^-$	191.0557	191.0561	2.14	$C_7H_{12}O_6$
	[caffeoyl] $^-$	179.0341	179.0350	4.90	$C_9H_8O_4$
4	$[M-H]^-$	515.1187	515.1195	1.55	$C_{25}H_{24}O_{12}$
	[M-H-caffeoyl] $^-$	353.0888	353.0878	-2.81	$C_{16}H_{18}O_9$
	[M-H-2caffeoyl] $^-$	191.0552	191.0561	4.75	$C_7H_{12}O_6$
	[caffeoyl] $^-$	179.0346	179.0350	2.12	$C_9H_8O_4$
	[caffeoyl-CO_2] $^-$	135.0448	135.0452	2.59	$C_8H_8O_2$
5	$[M-H]^-$	269.0458	269.0455	-0.94	$C_{15}H_9O_5$
	RDA fragmentation	151.0034	151.0037	1.86	$C_7H_4O_4$
	RDA fragmentation	117.0343	117.0346	2.44	C_8H_6O
6	$[M-H]^-$	283.0661	283.0671	3.42	$C_9H_{16}O_{10}$
	$[M-H-CH_3]^-$	268.0435	268.0436	0.35	$C_8H_{13}O_{10}$
	$[M-H-CH_3-CO]^-$	240.0477	240.0487	4.07	$C_7H_{13}O_9$
	RDA fragmentation	151.0036	151.0037	0.54	$C_7H_4O_4$
	RDA fragmentation	117.0348	117.0346	-1.79	C_8H_6O

1, chlorogenic acid; 2, luteolin-7-O-β-D-glucoside; 3, 3,5-dicaffeoylquinic acid; 4, 4,5-dicaffeoylquinic acid; 5, apigenin; 6, acacetin