Supplementary Material

Characterization, Classification and Authentication of Turmeric and Curry Samples by Targeted LC-HRMS Polyphenolic and Curcuminoid Profiling and Chemometrics

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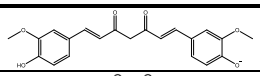
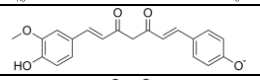
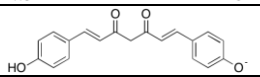
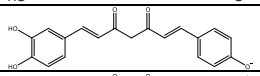
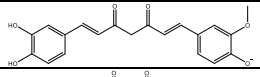
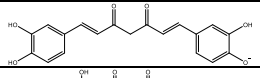
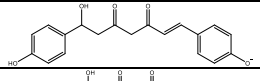
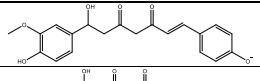
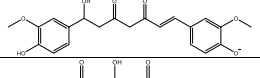
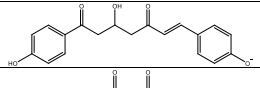
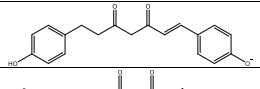
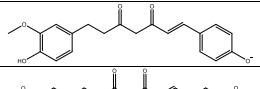
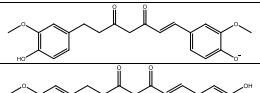
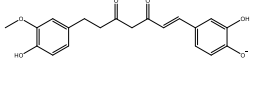
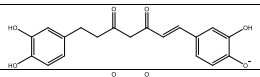
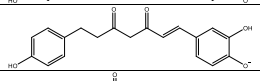
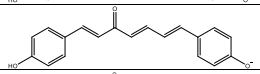
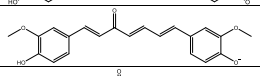
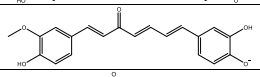
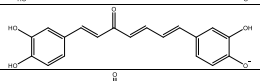
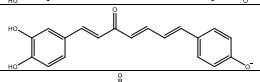
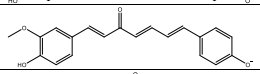
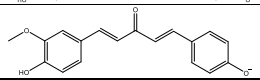
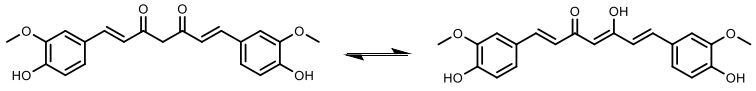
Table S1. HRMS curcuminoid accurate mass data base employed with TraceFinder™ software.

Compounds	Chemical formula	Tentative $[M-H]^-$ structure	$[M-H]^-$ *m/z* calculated value
curcumin	$C_{21}H_{20}O_6$		367.11869
Dmc	$C_{20}H_{18}O_5$		337.10812
bdmc	$C_{19}H_{16}O_4$		307.09756
5	$C_{19}H_{16}O_5$		323.09247
10	$C_{20}H_{18}O_6$		353.10304
N1	$C_{19}H_{16}O_6$		339.08739
1	$C_{19}H_{18}O_5$		325.10812
2 and 3	$C_{20}H_{20}O_6$		355.11869
6	$C_{21}H_{22}O_7$		385.12925
4	$C_{19}H_{18}O_5$		325.10812
9	$C_{19}H_{18}O_4$		309.11321
N2	$C_{20}H_{20}O_5$		339.12377
N3	$C_{21}H_{22}O_6$		369.13434
N4	$C_{20}H_{20}O_6$		355.11869

N5	$C_{19}H_{18}O_6$		341.10304
N6	$C_{19}H_{18}O_5$		325.10812
8	$C_{19}H_{16}O_3$		291.10264
N7	$C_{21}H_{20}O_5$		351.12377
N8	$C_{20}H_{18}O_5$		337.10812
N9	$C_{19}H_{16}O_5$		323.09247
N10	$C_{19}H_{16}O_4$		307.09756
N11	$C_{20}H_{18}O_4$		321.11321
7	$C_{18}H_{16}O_4$		295.09756

For most of the compounds, both keto and enol tautormes can be present as shown below:



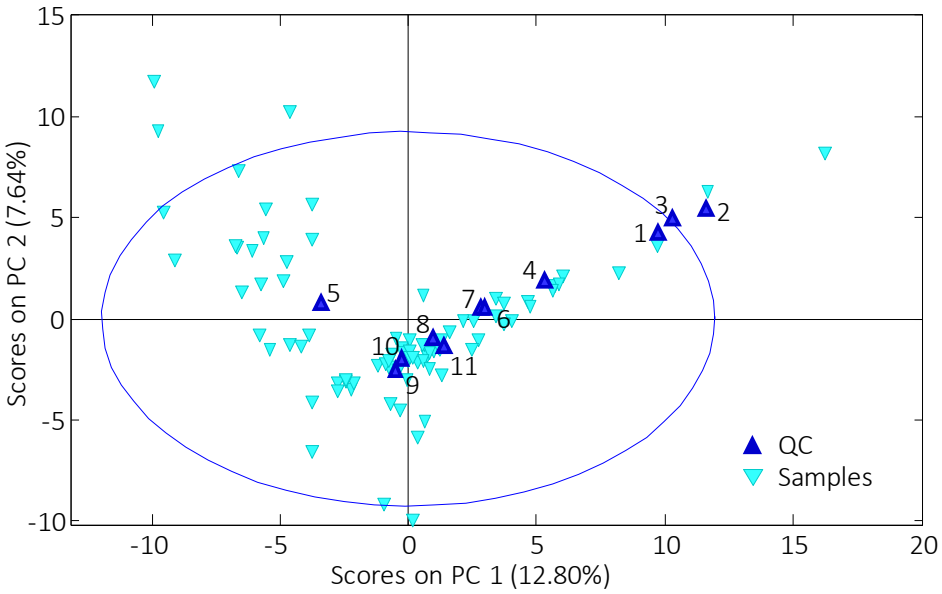
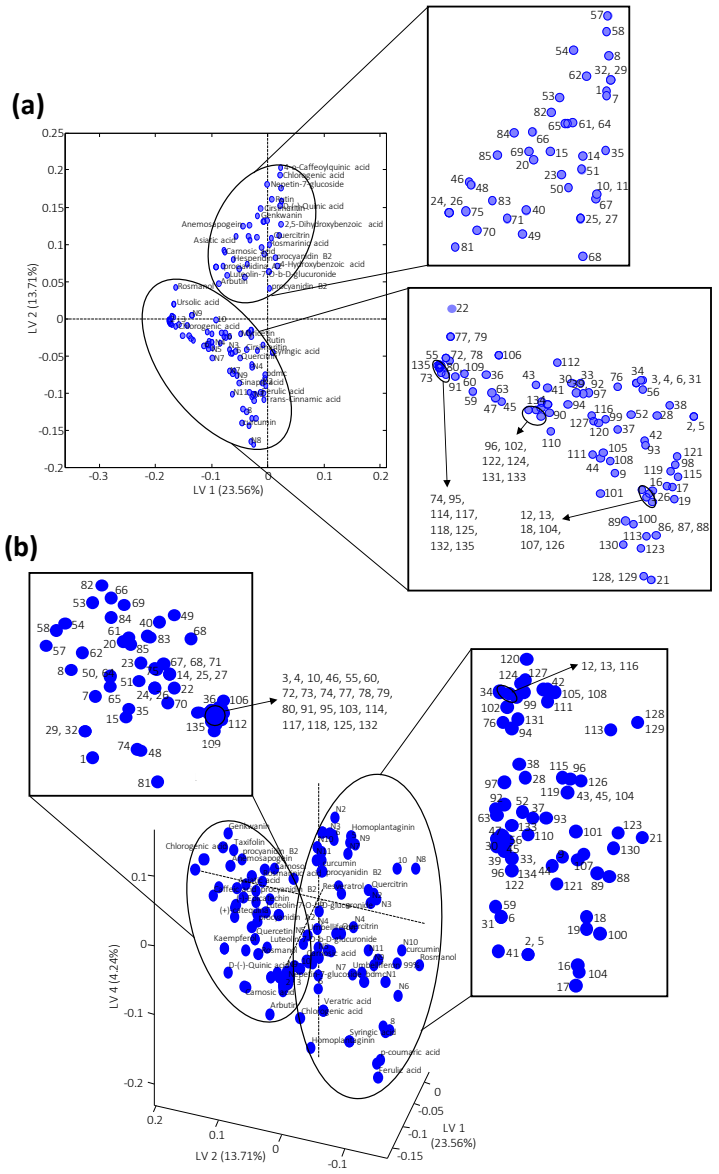


Figure S1. PCA score plot of PC1 vs. PC2 showing the behavior of QCs and analyzed samples when targeted LC-HRMS bioactive compound profiles were used as chemical descriptors. A total of 4 PCs were used to build the model.



	Variable	t_R
1	D-(-)-Quinic acid	3.01
2	Ethyl gallate	3.81
3	Homovanillic acid	3.81
4	Syringaldehyde	3.81
5	Syringic acid	3.81
6	Veratric acid	3.81
7	2,5-Dihydroxybenzoic acid	3.82
8	Caffeic acid	3.86
9	Sinapic acid	3.86
10	3,4-Dihydroxybenzaldehyde	4.32
11	4-Hydroxybenzoic acid	4.32
12	Homogentisic acid	4.36
13	Vanillic acid	4.36
14	Ellagic acid	4.49
15	Polydatin	4.58
16	*p*-coumaric acid	5.11
17	Ferulic acid	5.26
18	Vanillin	5.45
19	*trans*-Cinnamic acid	6.11
20	*trans*-Cinnamic acid	7.38
21	Rosmanol	6.55
22	Rosmanol	7.82
23	Rosmanol	10.55
24	Morin	4.01
25	Morin	7.12
26	Quercetin	4.01
27	Quercetin	7.12
28	Resveratrol	7.47
29	Fisetin	7.07
30	Fisetin	8.77
31	Fisetin	9.33
32	Kaempferol	7.07
33	Kaempferol	8.77
34	Kaempferol	9.33
35	Quercitrin	4,00
36	Quercitrin	4.69
37	Quercitrin	10.95
38	Quercitrin	11.49
39	Quercitrin	12.68
40	Homoplantaginin	4.5
41	Homoplantaginin	8.06
42	Homoplantaginin	11.45
43	Umbelliferon	11.67
44	Umbelliferon	13.33
45	12-methoxycarnosic acid	17.13
46	12-methoxycarnosic acid	19.54
47	Carnosic acid	17.13
48	Carnosic acid	19.58
49	Carnosol	18.07
50	Rosmarinic acid	3.83
51	Rosmarinic acid	4.81
52	Cirsimaritin	8.30
53	Cirsimaritin	10.87
54	Nepetin-7-glucoside	4.40
55	Nepetin-7-glucoside	10.36
56	Nepetin-7-glucoside	12.70
57	4-o-Caffeoylquinic acid	3.97
58	Chlorogenic acid	3.97
59	Chlorogenic acid	9.93
60	Chlorogenic acid	13.02
61	Gallic acid	3.79
62	Rutin	3.65
63	Rutin	12.61
64	(-)-Epicatechin	3.97
65	(+)-catechin	3.97
66	Taxifolin	5.03
67	Procyanidin B2	5.59
68	procyanidin B2	6.27
69	procyanidin B2	9.24
70	Luteolin-7-O-b-D-glucuronide	5.73
71	Luteolin-7-O-b-D-glucuronide	6.32
72	Luteolin-7-O-b-D-glucuronide	10.55
73	Luteolin-7-O-b-D-glucuronide	12.42
74	Luteolin-7-O-b-D-glucuronide	13.22
75	procianidina A2	3.03
76	Myricetin	5.46
77	Betulinic acid	23.17
78	Betulinic acid	25.46
79	Ursolic acid	23.17
80	Ursolic acid	25.46
81	Arbutin	3.02
82	Genkwanin	12.51
83	Hesperidin	3.96
84	Anemosapogein	19.43
85	Asiatic acid	13.03
86	1	6.41
87	4	6.41
88	N6	6.41
89	N1	6.86
90	N1	7.23
91	N4	7.92
92	N4	9.26
93	N4	10.89
94	N4	11.26
95	7	9.19
96	6	8.85
97	6	9.91
98	6	10.81
99	6	11.16
100	8	10.43
101	N11	10.68
102	N11	11.29
103	5	9.44
104	5	10.82
105	5	11.42
106	N9	9.44
107	N9	10.82
108	N9	11.38
109	N7	10.90
110	N7	11.44
111	N7	14.52
112	10	10.29
113	10	11.14
114	9	8.05
115	9	12.27
116	9	13.00
117	N2	8.03
118	N2	9.00
119	N2	12.54
120	N2	13.14
121	bdmc	12.80
122	bdmc	13.47
123	N10	12.70
124	N10	13.47
125	N3	8.67
126	N3	12.83
127	N3	13.61
128	dmc	13.21
129	N8	13.01
130	curcumin	13.47
131	curcumin	14.05
132	N5	5.89
133	N5	6.66
134	N5	7.49
135	2 i 3	2.89

Figure S2. Enlargment of loadings plot depitect in Figure 3 with full name descriptios. (a) LV1 *vs.* LV2 and (b) LV1 *vs.* LV2 *vs.* LV3 when using corrected targeted LC-HRMS polyphenolic and curcuminoid profiles as sample chemical descriptors.

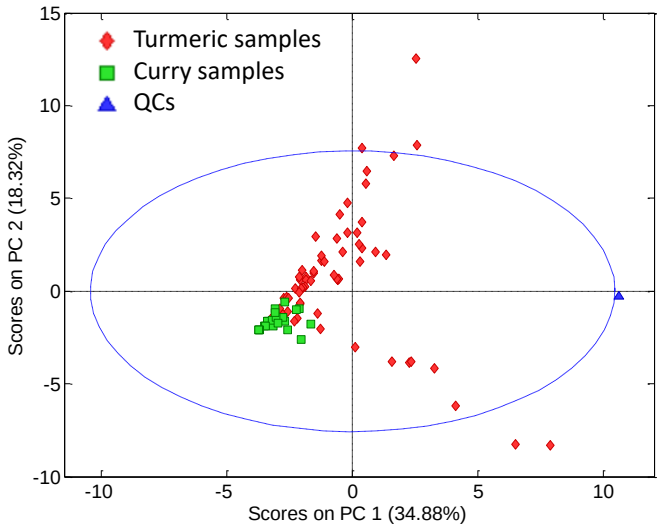


Figure S3. PCA score plot of PC1 vs. PC2 when only corrected targeted LC-HRMS curcuminoid profiles were used as sample chemical descriptors. A total of 4 PCs were employed to build the model.