

Lipid compositions and geographical discrimination of ninety-four geographically authentic wheat samples based on UPLC-MS with non-targeted lipidomic approach

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Table 1. Collection information of wheat samples used in this research.

Sample No.	Geographical origin (province)
1-16	Anhui
17-24	Fujian
25-29	Guizhou
30	Guangdong
31-41	Hubei
42-61	Henan
62-71	Gansu
72-94	Shaanxi

(All wheat samples were obtained in March 2018, China.)

Table 2. Identified discriminant markers according to the PLS-DA loadings with VIP > 1.5.

Marker No.	m/z	Compound	VIP	Highest abundance	Lowest abundance
1	855.74	TG (16:1/18:1/18:2)*	1.87	Anhui	Gansu
2	824.77	TG (16:0/16:0/16:0)	5.43		
3	850.79	TG (18:1/16:0/16:0)	4.04		
4	930.85	TG (18:1/18:1/20:1)	4.04	Anhui	Hubei
5	967.63	DGDG (18:0/18:2)	1.95		
6	876.80	TG (16:0/18:1/18:1)*	5.81		
7	777.55	MGDG (18:2/16:0)*	2.6	Fujian	Gansu
8	518.32	Lyso PC (18:3)*	1.62	Fujian	Hubei
9	496.34	Lyso PC (16:0)*	4.82	Gansu	Guizhou
10	894.75	TG (18:3/18:2/18:2)*	6.48		
11	641.51	DG (18:2/18:1)	4.04		
12	801.55	MGDG (18:2/18:2)	3.55		
13	870.75	TG (18:3/18:2/16:0)	5.59		
14	780.55	PC (18:2/18:3)	3.8		
15	799.53	MGDG (18:3/18:2)	2.26		
16	782.57	PC (18:2/18:2)	5.88		
17	756.55	PC (16:0/18:3)	2.66	Gansu	Hubei
18	740.52	PE (18:2/18:2)	2.61		
19	784.59	PC (18:2/18:1)	4.33		
20	758.57	PC (16:0/18:2)	5.37		
21	716.52	PC (18:2/13:0)	1.82		
22	786.60	PC (18:1/18:1)	3.89		
23	941.62	DGDG (18:1/16:0)	1.9		
24	760.59	PC (16:0/18:1)	4.32		
25	734.57	PC (16:0/16:0)	1.78		

26	575.50	DG (18:2/16:0)	4.62		
27	892.74	TG (18:2/18:3/18:3)	3.15		
28	868.74	TG (16:0/18:3/18:3)	1.95		
29	926.82	TG (20:1/18:2/18:2)	3.27		
30	848.77	TG (18:2/16:0/16:0)	5.32		
31	954.85	TG (18:2/22:1/18:2)	2.02		
32	928.83	TG (18:2/18:1/20:1)	2.98		
33	982.88	TG (24:1/18:2/18:2)*	1.88	Henan	Hubei
34	279.23	Linolenic acid	2.04	Hubei	Gansu
35	263.24	Linoleic acid*	3.76		

VIP represents variable influence on projection.

Compounds marked with * were those with maximum VIP value of the corresponding province group set.

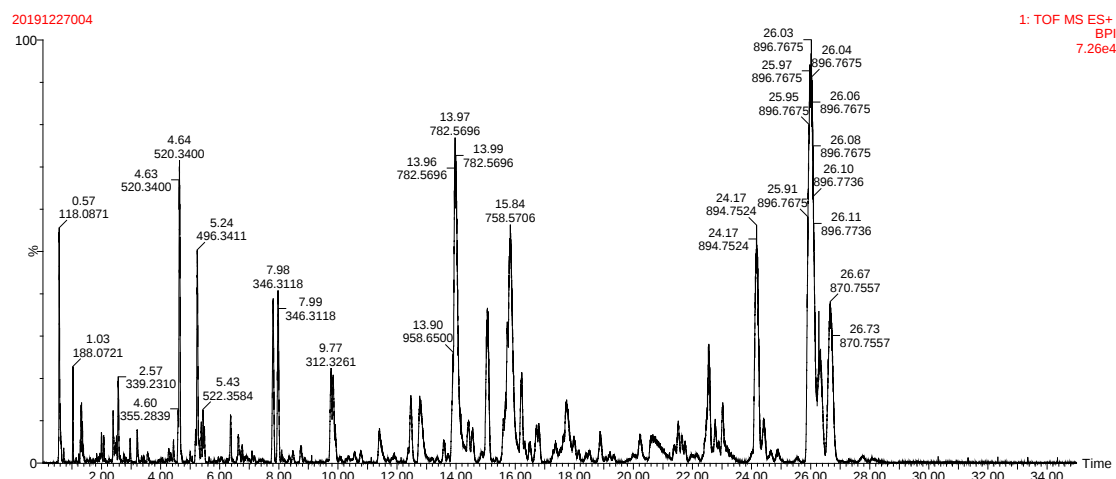


Figure 1. Base peak intensity chromatogram of QC sample only extracted by dichloromethane/methanol (5/5, v/v).

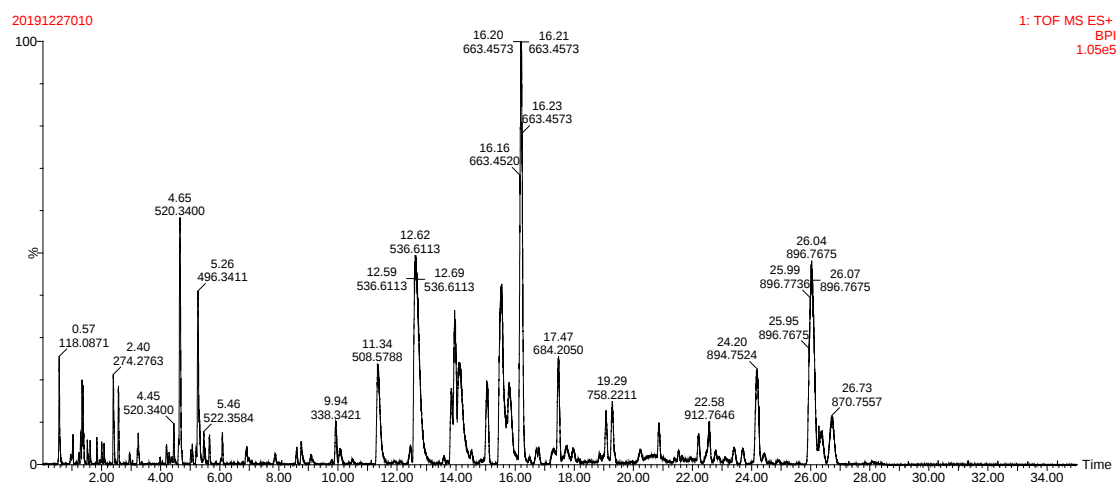


Figure 2. Base peak intensity chromatogram of QC sample merged the 3-step extractions (n-hexane - dichloromethane/methanol (5/5, v/v) - acetone/water (5/5, v/v)).

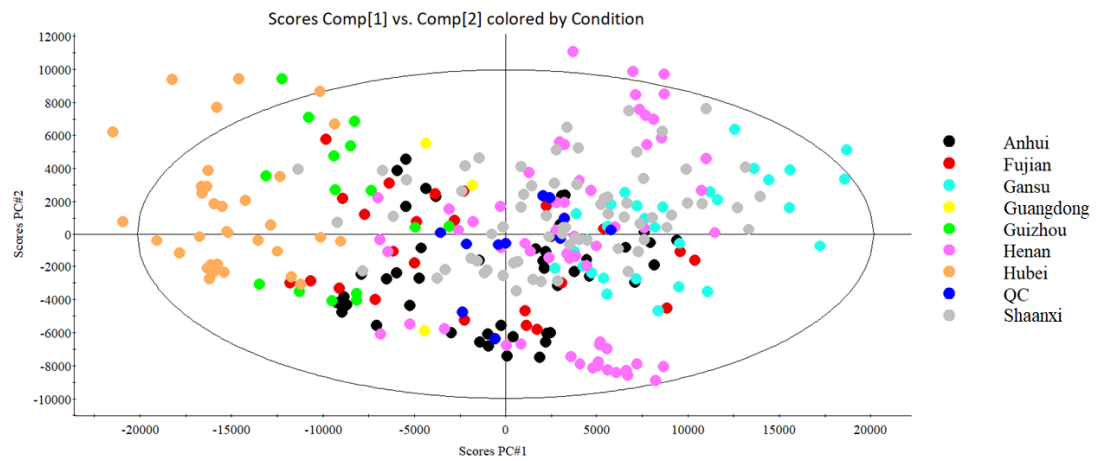


Figure 3. Principal component analysis (PCA) scores plot of wheat samples from 8 provinces in China, including 3771 variables without any filtrations.

