One class classification based authentication of peanut oils by fatty acid profiles

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Supporting material 1: Experimental section

1.1 Materials and regents

To ensure that the oil samples could represent the actual status of edible oils, 80 peanut samples were collected from different product areas and employed to prepare edible oils by oil mill machinery (TZC-0502, Brand of TEN GUARD, China). Supelco 37 component FAME mix (No. 47885-U) was purchased from Sigma (St. Louis, MO, USA). 11-octadecenoic acid (C18:1n-7, >97.0 purity) and 7-hexadecenoic acid methyl ester were purchased from Sigma (St. Louis, MO, USA).

1.2 Experimental procedure of derivatization

As descried in the previous study^{1, 2}, 0.06g of vegetable oil sample was diluted with 2 mL solvent of diethyl ether and petroleum ether (v/v 1:1) and 1mL 0.4M KOH-CH₃OH was added, vortex-mixed for 30s and placed at room temperature for 2.5h, and then, 2ml redistilled water was added, vortexmixed, centrifuged at 4500 rpm for 2 min. 200 μ L of the organic phase was collected and diluted by 800 μ L petroleum ether, prior to analysis by GC-MS.

1.3 Fatty acid analysis

According to the previous study^{1,2}, the analyses were performed by Agilent GC-7890 gas chromatograph interfaced to a Agilent 5973 mass spectrometer. In the gas chromatography system, a fused silica capillary column DB-23 ($30 \text{ m} \times 0.25 \text{ mm}$ i.d. $0.15 \mu \text{m}$ film) (Agilent Technologies) was used. Helium (99.999% purity) was used as carrier gas at a flow-rate of 1.2 mL min⁻¹. The column was first set at 100 °C and held for 0.2 min, temperature was subsequently increased to 215°C at the rate of 10 °C/min and held for 0.1min, finally to 224 °C at the rate of 2°C/min, which was held for an

additional 0.2 min (total program time, 16.5min). This is the optimum temperature programming for the conditions of both separation effect and run time. Mass spectrometric conditions were as follows: ionization mode: EI; electron energy 70eV; temperatures of injector, ion-source and detector at 220, 250 and 150 °C, respectively. Solvent cut time was 3 min. Splitting ratio was 20:1. Selected ion monitoring (SIM) mode: m/z 55, 67, 74 and 79.

Identification of fatty acids in SIM mode was conducted according to the protocol in our previous study²⁵. Fatty acid percentage composition (percentage of peak area) was employed as quantitative results for edible oils.

[1] L.X. Zhang, P.W. Li, X.M. Sun, X.F. Wang, B.C. Xu, W.P. Wang, F. Ma, Q. Zhang, X.X. Ding,
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[2] L.X. Zhang, P.W. Li, X.M. Sun, W. Hu, X.P. Wang, Q. Zhang, X.X. Ding, Untargeted fatty acid profiles based on the selected ion monitoring mode. Anal. Chim. Acta 839 (2010) 44-50.

Oil seeds	Geographical origin	Crop year	Oil seeds	Geographical origin	Crop year
Peanut seed 1-2	Henan, China	2013	Peanut seed 38-41	Hebei, China	2013
Peanut seed 3-4	Shandong, China	2012	Peanut seed 42-43	Heilongjiang, China	2013
Peanut seed 5-8	Hebei, China	2013	Peanut seed 44-47	Jiangsu, China	2013
Peanut seed 9-10	Heilongjiang, China	2013	Peanut seed 48-50	Zhejiang, China	2013
Peanut seed 11-13	Jiangsu, China	2013	Peanut seed 51-55	Yunnan, China	2013
Peanut seed 14-17	Guangdong, China	2013	Peanut seed 56-60	Liaoning, China	2013
Peanut seed 18-20	Guangxi, China	2013	Peanut seed 61-65	Zhejiang, China	2013
Peanut seed 21-25	Hubei, China	2013	Peanut seed 66-68	Hunan, China	2013
Peanut seed 26-30	Hunan,China	2013	Peanut seed 69-71	Guangxi, China	2013
Peanut seed 31-33	Fujian, China	2013	Peanut seed 72-75	Hubei, China	2013
Peanut seed 34-35	Henan, China	2013	Peanut seed 76-78	Henan, China	2013
Peanut seed 36-37	Shandong, China	2013	Peanut seed 79-80	Shandong, China	2013

Supporting material Table S1 Detailed information of peanuts used in this study

FAME	Retention Times	ECL	ECL in Database ^a
12:0	5.689	12.000	12.000
14:0	7.422	14.000	14.000
15:0	8.260	15.000	15.000
15:1 n-5c	8.581	15.388	15.420
16:0	9.088	16.000	16.000
16:1 n-9c	9.298	16.216	16.220
16:1 n-7c	9.352	16.272	16.331
16:1 n-5c	9.429	16.351	16.383 b
16:2 n-5c	9.803	16.736	16.677 b
17:0	10.059	17.000	17.000
17:1 n-7c	10.253	17.340	17.341
18:0	10.630	18.000	18.000
18:1 n-9c	10.832	18.290	18.265
18:1 n-7c	10.862	18.333	18.359
18:1 n-x	11.092	18.663	_c
18:2 n-6c	11.187	18.780	18.764
18:3 n-6c	11.441	19.164	19.093
19:1 n-8	11.484	19.226	<i>19.218</i> b
18:3 n-3c	11.590	19.378	19.436
20:0	12.023	20.000	20.000
20:1 n-9c	12.221	20.264	20.278
20:2 n-6c	12.623	20.801	20.843
21:0	12.772	21.000	21.000
22:0	13.443	22.000	22.000
22:1 n-9c	13.843	22.261	22.302
23:0	14.550	23.000	23.000
24:0	15.609	24.000	24.000
24:1 n-9c	15.983	24.353	24.353

Supporting material Table S2 Identification of FAMEs in peanut oils

^a ECL values in Database in Ref. 14

^b ECL values in Chrombox database (Lib_Z_BP-20)

^c no closed ECL and possible structure is deduced by mass spectral characteristics