

Supporting Information

Statistical Evaluation of Triacylglycerol Composition in Plant Oils Based on High-Performance Liquid Chromatography - Atmospheric Pressure Chemical Ionization Mass Spectrometry Data

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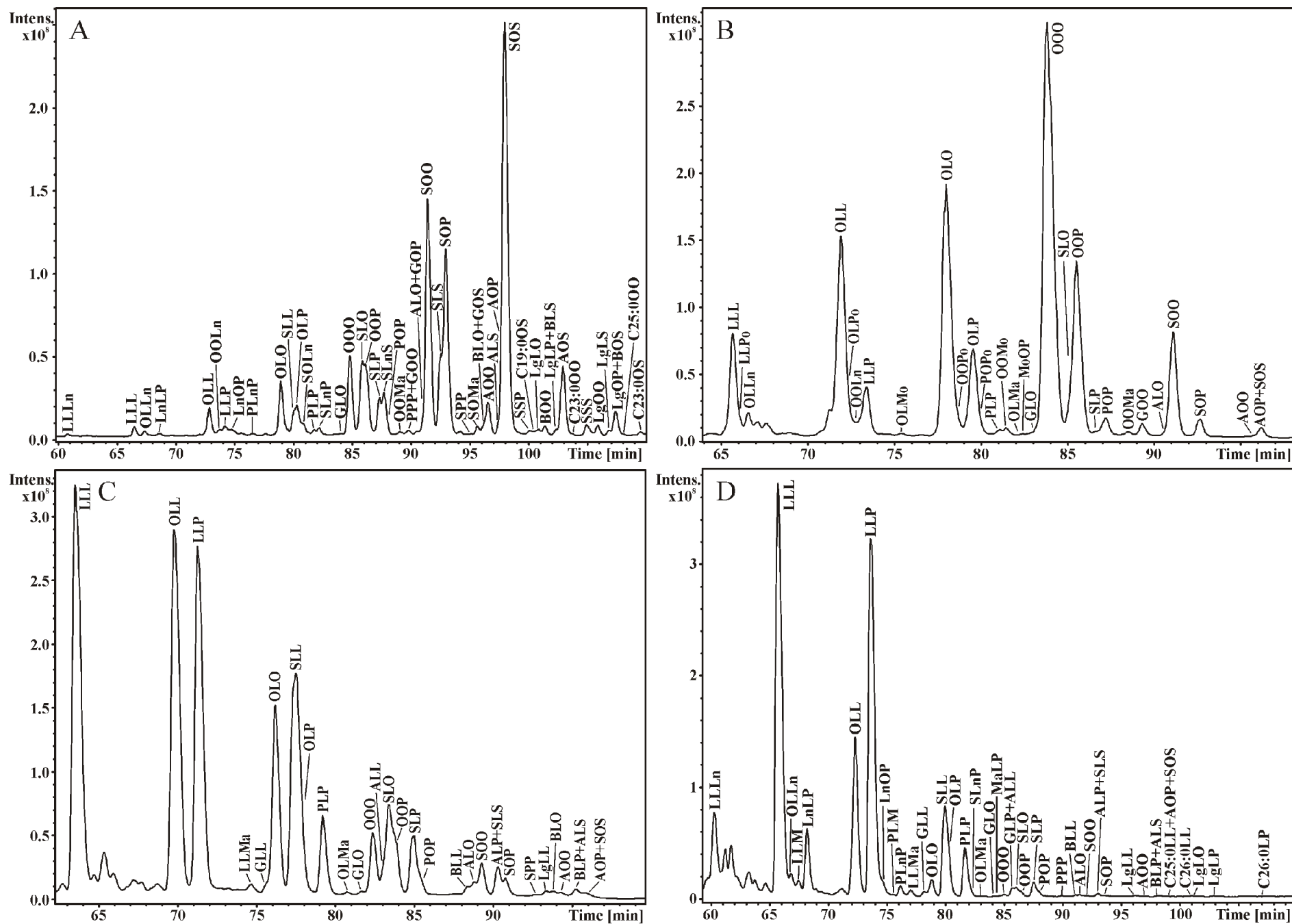


Figure S1. NARP-HPLC/APCI-MS analysis of plant oils: (A) mango (*Mangifera indica*), (B) hazelnut (*Corylus avellana*), (C) pumpkin (*Cucurbita pepo*) and (D) cucumber (*Cucumis sativus*).

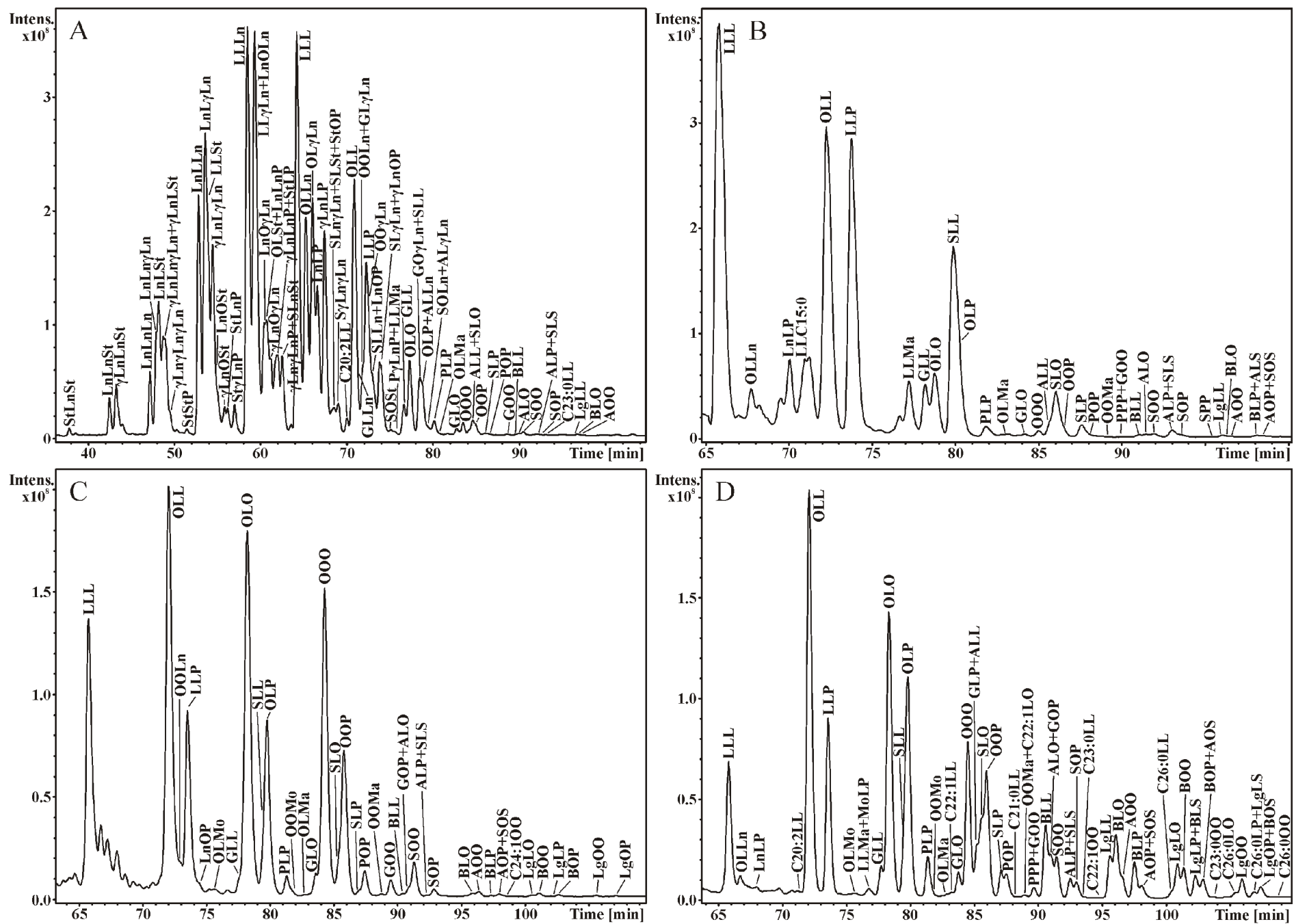


Figure S2. NARP-HPLC/APCI-MS analysis of plant oils: (A) blackcurrant (*Ribes nigrum*), (B) melon cantaloupe (*Cucumis melo cantalupensis*), (C) pistachio (*Pistacia vera*) and (D) peanut (*Arachis hypogaea*).

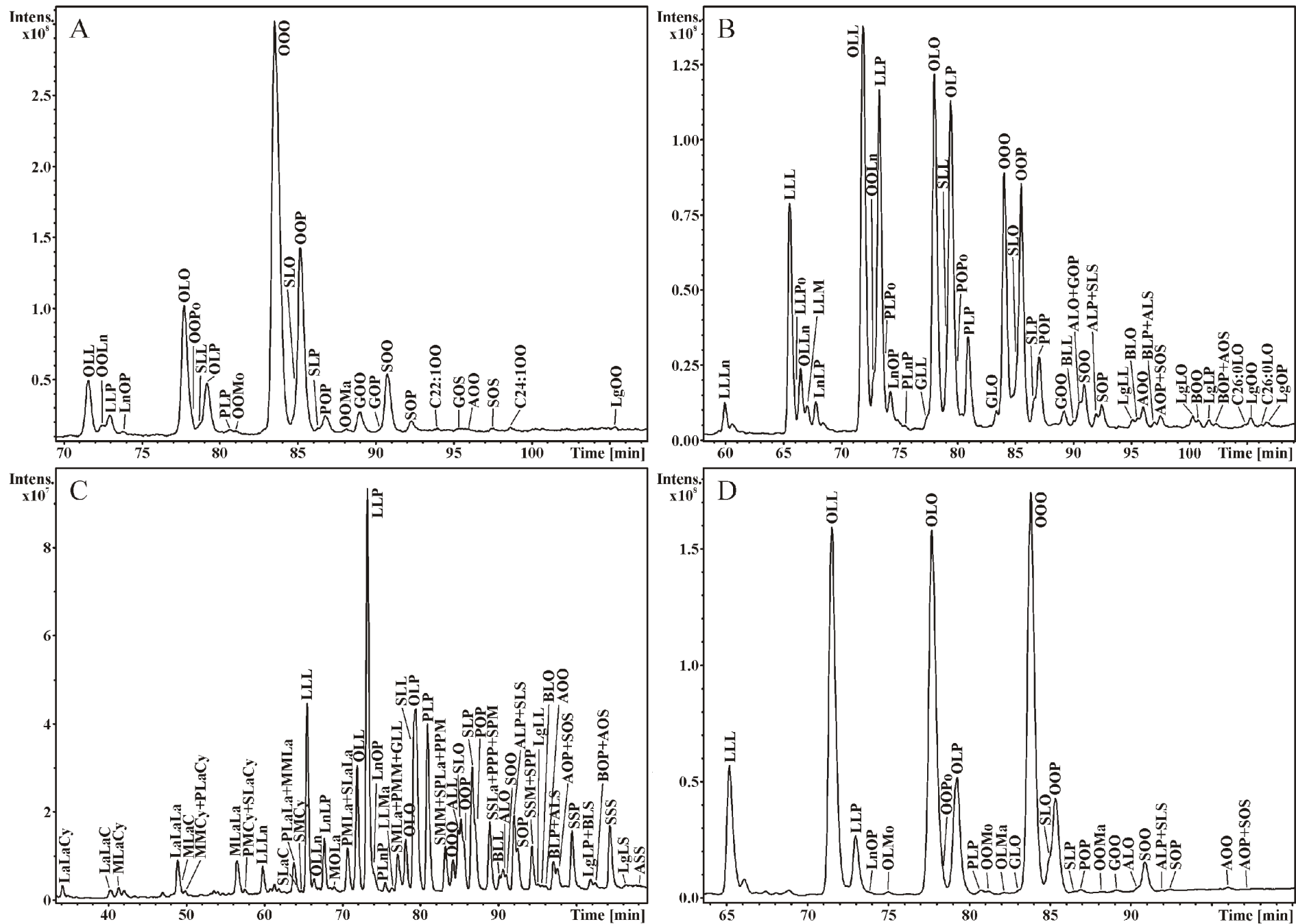


Figure S3. NARP-HPLC/APCI-MS analysis of plant oils: (A) camellia (*Camellia sinensis*), (B) rice (*Oryza sativa*), (C) coffee butter and (D) apricot kernel (*Prunus armeniaca*).

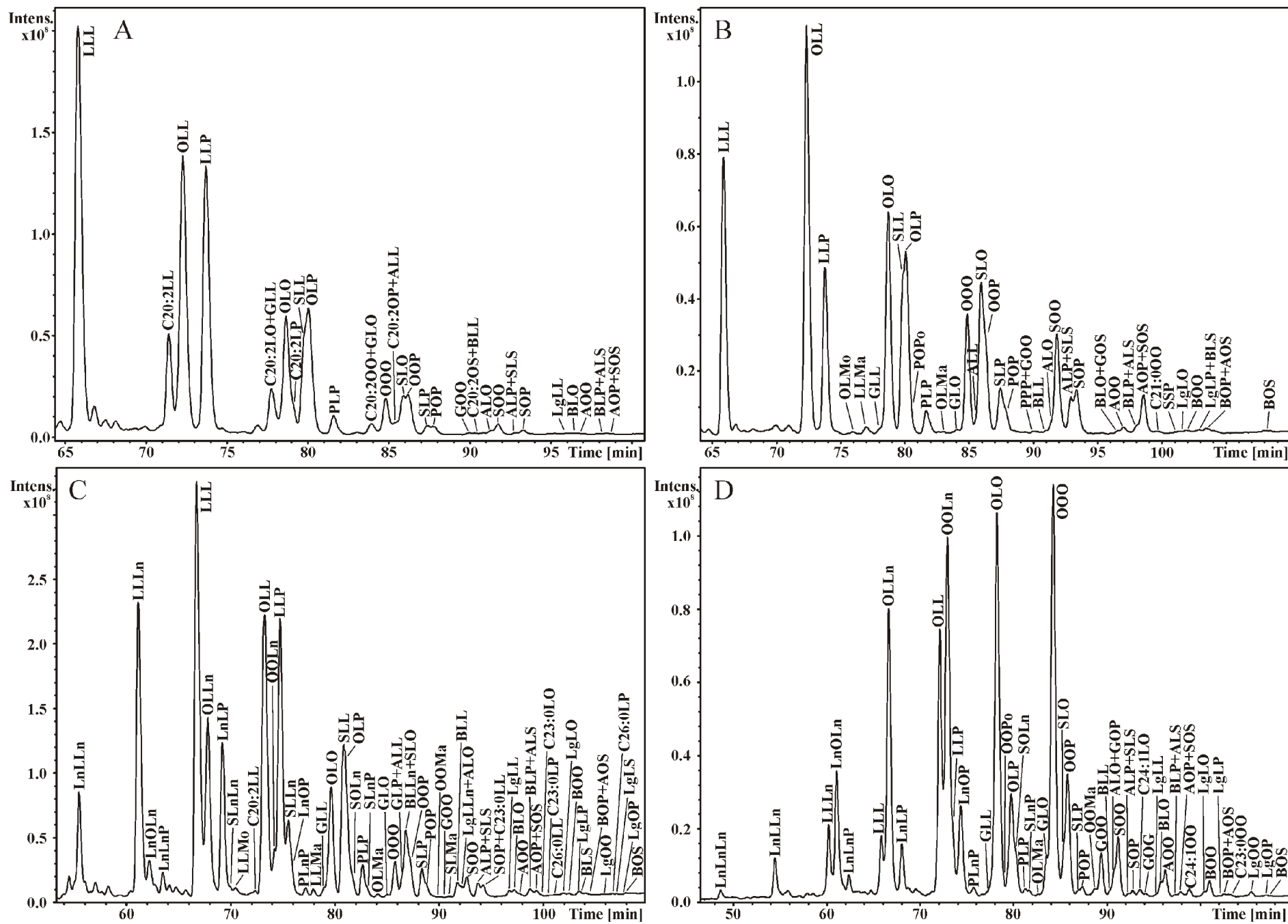


Figure S4. NARP-HPLC/APCI-MS analysis of plant oils: (A) black cumin (*Nigella sativa*), (B) tamanu (*Calophyllum tacamahaca*), (C) soya (*Glycine max*) and (D) rapeseed (*Brassica napus*).

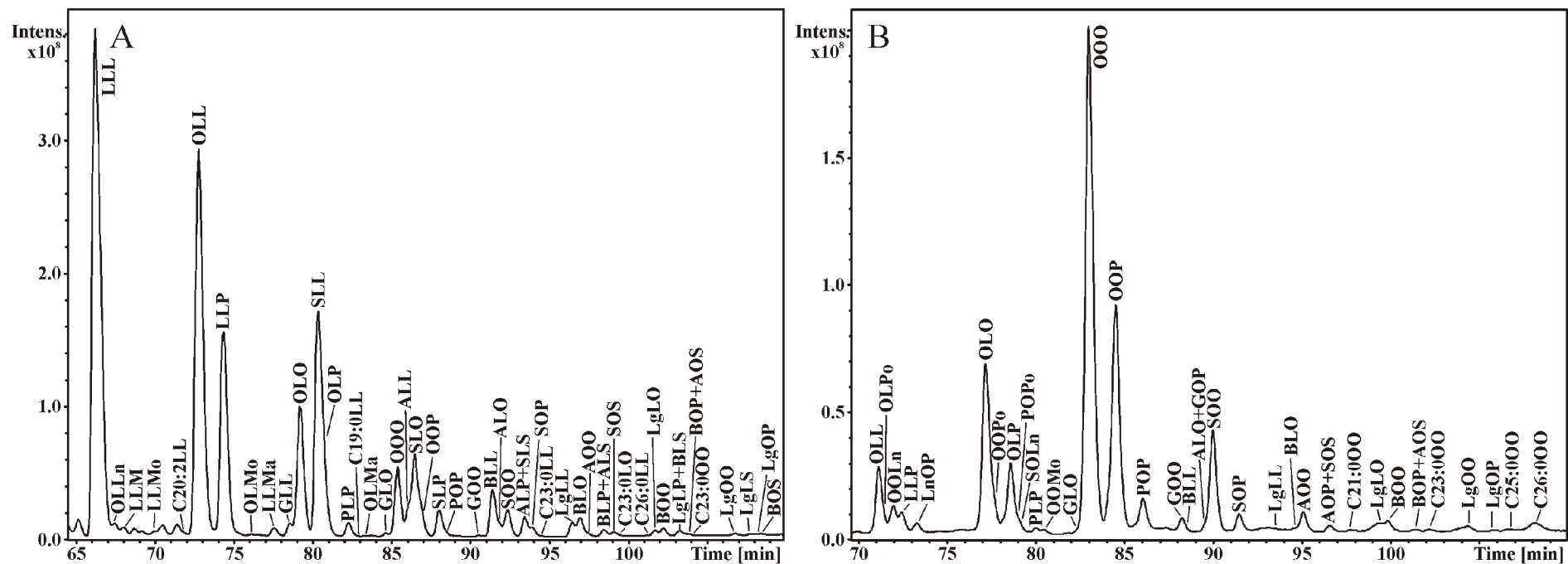


Figure S5. NARP-HPLC/APCI-MS analysis of plant oils: (A) sunflower (*Helianthus annuus*) and (B) olive (*Olea europaea*).

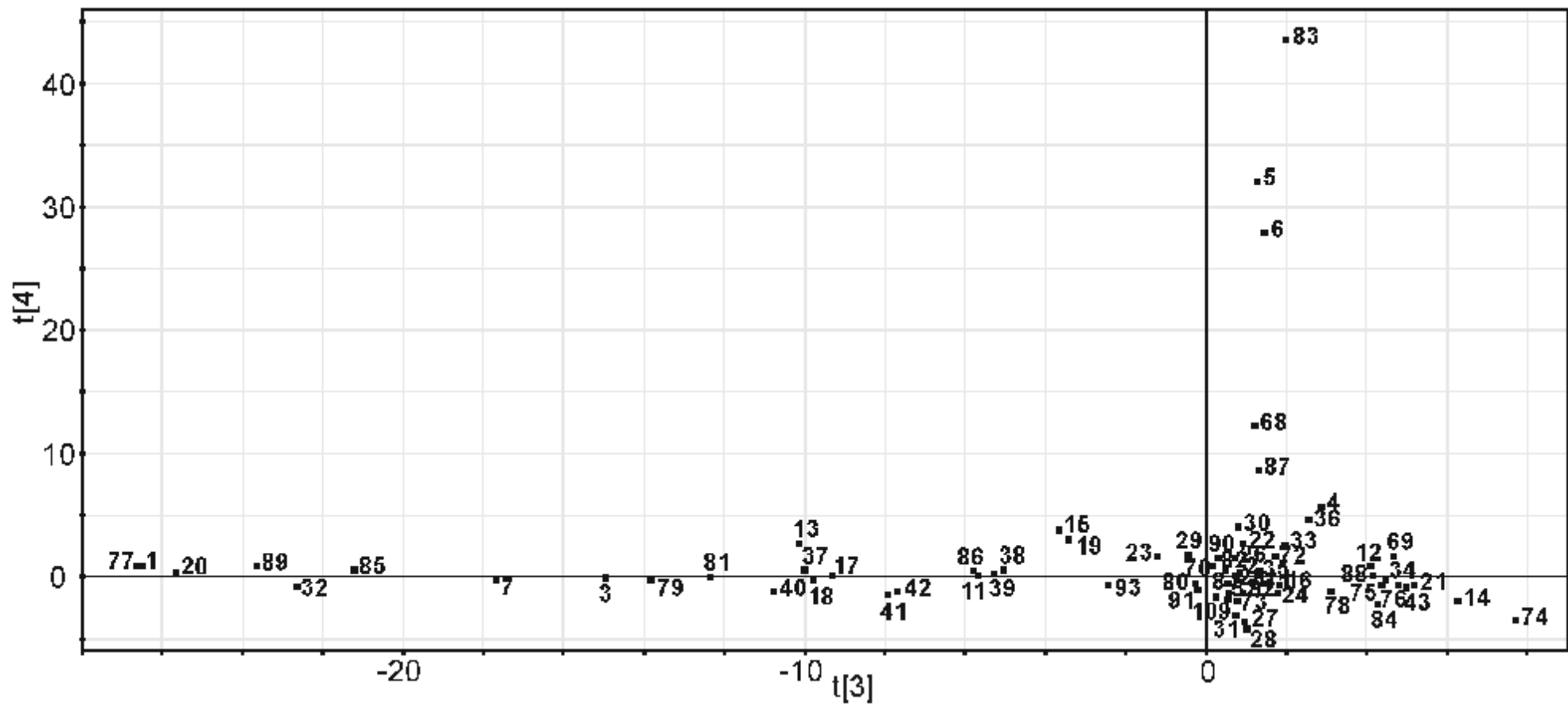


Figure S6. Projection of principal components $t[3]$ and $t[4]$ in two dimensional scatter plot for all measured samples. Numbers of individual plant oils are listed in Experimental part.

GLO	83.1		0.1		0.2		<0.1	0.2	0.1	0.2	0.4	0.1	0.1		<0.1	<0.1	0.1	<0.1	0.1	0.2	2.5	0.5	0.7			0.3		0.1	<0.1	0.2	0.3		0.1				
C22:1OLn	83.4		0.1																																		
GOPo	83.7			2.3																																	
OOO	84.0		0.5	17.0	0.7	6.8	7.5	2.4	35.2	36.9	12.3	3.5	4.4	0.2	2.6	0.2	0.4	3.0	1.7	0.3	31.6	6.5	17.7	8.2	47.8	51.1	10.7	0.7	28.8	1.0	14.3	3.1	35.1	7.2			
C20:2OP	84.6																														0.3						
GLP	84.7														0.2	0.1		0.2				1.0		0.5													
ALL	84.8			1.0	<0.1		0.9			0.4	0.6	0.2	0.5	0.3	0.3	<0.1	0.3	<0.1	0.3		0.7		0.6				0.7		0.3		0.2		0.7				
BLLn	85.1			0.7																									0.2								
SLO	85.1		0.5		0.6	4.8	4.3	1.5	2.2	2.7	0.6	3.0	1.8	0.8	1.4	0.5	0.3	1.7	0.3	2.2	1.7	1.3	1.4	1.9	0.4	0.2	3.0	1.3	1.1	0.2	2.5	2.0	0.8	6.2			
OOP	85.4		0.6	8.6	0.8	7.8	6.6	0.9	11.4	12.1	9.3	3.1	5.9	0.6	6.0	0.4	0.3	4.9	1.2	1.0	22.1	7.4	8.3	7.4	18.6	17.0	7.4	1.2	7.0	0.5	12.0	3.4	10.3	4.6			
AOLn	85.5			0.1																																	
SOPo	85.6			3.5																																	
SLP	86.6		<0.1		0.1	2.8	2.1	0.1	0.3	0.3	0.3	2.5	1.3	0.6	2.0	0.9	<0.1	2.0	<0.1	0.7	0.4	0.4	0.1	0.9	0.2	0.1	0.5	2.8	0.1	0.1	1.1	0.6		2.3			
SLnS	86.9					0.5	0.1																														
POP	87.0			2.2	0.1	3.4	2.5	<0.1	1.4	1.2	1.9	1.1	2.8	0.4	4.2	0.4	<0.1	3.0	0.1	0.2	6.3	1.8	1.5	1.3	2.2	1.8	3.5	1.8	0.2	<0.1	3.0	0.8	1.1	1.6			
SSLa	88.7																																	1.6			
PPP	88.7		<0.1				0.1				0.1		<0.1	<0.1		0.1					<0.1				0.1								1.2		<0.1		
SPM	88.9																																		0.7		
C21:0LL	87.4				<0.1			<0.1							<0.1																				<0.1		
C23:0LLn	87.8				<0.1			<0.1																												<0.1	
OOMa	88.4						0.3		0.3	0.3	0.1		0.1					<0.1		<0.1	0.5	0.1	0.1	<0.1	0.2	0.2			<0.1		0.1		0.2				
MaOP	89.7																					0.2															
C24:1LL	87.9				<0.1																																
C22:1LO	88.6																																			0.1	<0.1
GOO	89.0		<0.1	3.4	<0.1		0.3	0.1	0.6	0.6	0.5		<0.1				<0.1		<0.1	<0.1	1.0	1.7	0.6	0.3	1.5	1.4	0.5		0.1	<0.1	0.4	0.1	4.4	<0.1			
GLS	89.9																																			<0.1	
C20:2OS	89.9																																			<0.1	
BLL	9				0.4			0.2			0.2	0.2	<0.1	0.5	<0.1	<0.1	<0.1	0.1		0.1		1.3	<0.1	2.1		0.1	0.2		0.1	0.1	<0.1		<0.1				
LgLLn	90.2				0.1																																
ALO	90.4		<0.1	0.3	0.5	0.1	0.1	0.5	0.1	0.2	0.1	0.3	0.2	0.1	0.1	0.1	<0.1	0.2	<0.1	0.1	0.2	1.1	0.1	0.7			0.2	0.4	0.1	0.2	0.1	0.2		0.2			
GOP	90.4			0.8			0.2				0.2											0.8	0.9	0.1	0.7	0.1	0.1	0.4				0.2		1.8			
SOO	90.8		<0.1	3.0	0.4	5.2	21.0	0.5	5.3	6.2	1.0	1.3	1.5	0.1	0.8	0.1	0.1	0.9	0.2	0.2	6.5	1.3	1.5	1.8	4.7	5.1	1.4	0.3	1.6	0.2	4.6	0.8	8.4	5.5			
AOPo	91.0			3.3																																	
ALP	91.8				<0.1	<0.1		0.1			0.1	0.4	0.1	0.2	0.2	0.1	<0.1	0.2		<0.1	<0.1	0.2	<0.1	0.4			0.2	0.8	<0.1	<0.1	0.1	<0.1		0.2			

SLS	91.9		0.1		<0.1	0.9	1.8	0.1			<0.1	0.5	0.1	0.1	0.2	0.1	<0.1	0.2		0.3	<0.1	0.1	<0.1	0.3			0.1	0.6	<0.1	<0.1	0.2	<0.1		1.0		
SOP	92.3		0.1	1.2	0.1	3.7	14.0	0.1	1.0	1.2	0.2	0.7	1.2	0.1	1.0	0.1	<0.1	0.9	<0.1	0.2	3.1	0.5	0.3	0.6	0.8	0.9	0.9	1.1	0.1		2.3	0.4	1.6	3.1		
AOM	92.3		0.5																																	
SSM	94.4																											0.8								
SPP	94.4					<0.1						0.1							<0.1									0.7								
C23:0LL	92.4	51			<0.1			<0.1			0.1			0.1			<0.1					0.1		0.1						<0.1						
C21:0LO	93.0									<0.1													<0.1								<0.1					
C19:0OO	93.5																																	0.1		
C21:0LP	94.4										<0.1																									
SOMa	95.0						0.5																													
GOG	93.9	52		0.2							<0.1												<0.1											0.1		
C22:10O	94.0			0.3																					0.1	<0.1		<0.1	0.1	0.1				<0.1	0.2	
LgLL	94.9				0.2			0.1				0.1	0.1	0.1	0.4	0.1	<0.1	<0.1	0.2		0.1		0.8		0.9			0.2	0.1		<0.1	<0.1	<0.1			
BLO	95.5				0.2		0.1	0.1				0.1	0.2	0.1	0.1			<0.1	0.1		<0.1	0.1	1.8	0.1	2.4			0.2	0.1		0.1	<0.1	<0.1	0.2	<0.1	
GOS	95.7			0.4			0.3																0.1				0.1	<0.1					0.1		0.6	0.1
AOO	96.0			<0.1	2.6	0.2	0.1	2.0	0.2	0.5	0.5	0.2	0.1	0.1			<0.1	<0.1	0.1	<0.1	<0.1	0.9	0.9	0.2	0.7	0.2	0.1	0.6	0.1	0.1	<0.1	0.5	<0.1	6.8	0.4	
BOPo	96.1			1.5																																
BLP	96.8							<0.1				0.1	0.1	<0.1	0.2	<0.1	<0.1		0.1		<0.1	<0.1	0.6	<0.1	1.4			0.1	0.3		<0.1	<0.1	<0.1		0.1	
ALS	96.9					<0.1	0.1	<0.1					0.1	<0.1	0.1	<0.1	<0.1		<0.1		<0.1	<0.1					<0.1	0.2		<0.1	<0.1	<0.1			0.2	
LgLnP	97.1													<0.1																						
AOP	97.5			0.7			0.2		<0.1	<0.1			0.1	0.2	0.1	0.1	<0.1		0.1		<0.1	0.4	0.2	<0.1	0.3			0.2	0.2	<0.1	<0.1	0.2	<0.1	0.9	0.3	
SOS	97.6			0.1	0.7		1.6	18.4		<0.1	<0.1		0.1	0.1	<0.1	0.1	<0.1		0.1		<0.1	0.6	0.2	<0.1	0.2	0.1	0.2	0.2	0.2	<0.1	<0.1	0.5	<0.1	0.9	1.8	
BPoP	97.6			0.1																																
SSP	99.7					0.3																							1.5						<0.1	
C25:0LL	97.4	53													<0.1	<0.1		<0.1																		
C23:0LO	97.9																																			
C21:0OO	98.4																							<0.1	<0.1									0.2	<0.1	
C23:0LP	99.5															<0.1	<0.1	<0.1						<0.1												
C19:0OS	100.2					0.1																														
C24:10O	98.9	54																					<0.1	<0.1	<0.1		<0.1	<0.1				<0.1				
C26:0LL	100.1				<0.1									0.1		<0.1		<0.1									0.1					<0.1				
LgLO	100.5				0.1		0.2							0.1	0.1	<0.1	<0.1		0.1				<0.1	1.1	<0.1	1.2			0.3		<0.1	0.1			0.1	
AOG	100.7			0.2																																
BOO	101.0			1.3	0.1		0.6									<0.1										0.4	1.1	0.1	1.3			0.2			0.1	13.2

Table S3. Relative weight concentrations [%] of individual fatty acids in soya, rapeseed, sunflower and olive cooking oils and in four samples of adulterated olive oil by 1, 2, 5 or 10% of sunflower oil (Olive/Sunflower) calculated from HPLC/APCI-MS of triacylglycerols

Oil	No.	M	P	Po	Ma	Mo	S	O	L	Ln		A	G			B		Lg			
		C14:0	C16:0	C16:1	C17:0	C17:1	C18:0	C18:1	C18:2	C18:3	C19:0	C20:0	C20:1	C20:2	C21:0	C22:0	C23:0	C24:0	C24:1	C25:0	C26:0
Soya	38		12.0		0.05	0.03	3.3	26.3	49.8	7.2		0.4	0.1	0.01		0.5	0.1	0.2			0.01
	39		11.5		0.04	0.04	3.3	25.3	50.8	7.7		0.4	0.1	0.01		0.5	0.1	0.2			0.01
Rapeseed	41		7.0	0.2	0.1		1.6	58.2	21.3	9.6		0.4	1.1			0.3	0.03	0.1	0.07		
	42		7.2	0.2	0.07		1.6	57.9	21.9	9.1		0.4	1.0			0.3	0.03	0.2	0.1		
Sunflower	44	0.3	7.6		0.06	0.08	3.8	24.6	61.5	0.4	<0.01	0.4	0.1	<0.01		0.8	0.05	0.3			0.01
	45	0.2	7.7		0.03	0.03	3.2	22.3	64.8	0.1	<0.01	0.3	0.1	0.01		0.9	0.02	0.3			0.01
	46	0.2	8.4		0.03	0.04	3.1	23.7	62.8	0.2	<0.01	0.3	0.1	<0.01		0.8	0.02	0.3			0.01
	47	0.3	8.3		0.03	0.04	3.4	24.7	61.4	0.3	<0.01	0.3	0.1	<0.01		0.8	0.03	0.3			<0.01
	48	0.2	8.0		0.05	0.05	3.1	25.0	62.0	0.06	<0.01	0.3	0.1	<0.01		0.8	0.04	0.3			<0.01
	49	0.2	7.9		0.03	0.02	3.2	22.7	64.4	0.03	<0.01	0.3	0.1	<0.01		0.8	0.02	0.3			<0.01
	50	0.2	7.9		0.07	0.04	3.3	23.3	63.6	0.05	<0.01	0.3	0.1	<0.01		0.8	0.03	0.3			0.01
51	0.2	8.2		0.05	0.06	3.9	24.6	61.3	0.05	<0.01	0.3	0.1	<0.01		0.9	0.04	0.3			<0.01	
Olive	53		12.6	1.2		0.1	2.3	74.9	6.5	1.0		0.5	0.4		0.02	0.3	0.05	0.1		0.02	0.01
	54		12.3	1.0		0.07	3.1	77.1	4.5	0.8		0.5	0.3		0.01	0.2	0.03	0.07		0.01	0.01
	55		13.2	1.2		0.09	2.7	72.2	8.7	0.9		0.5	0.2		0.01	0.2	0.02	0.07		0.01	<0.01
	56		11.6	1.2		0.1	2.7	73.2	9.0	0.9		0.5	0.3		0.02	0.3	0.05	0.1		0.02	0.01
	57		11.8	1.2		0.1	3.2	77.3	4.3	1.0		0.5	0.3		0.01	0.2	0.02	0.05		0.01	0.01
	58		13.9	1.3		0.1	2.9	71.0	8.8	0.9		0.5	0.3		0.01	0.2	0.02	0.05		0.01	0.01
	59		12.2	1.2		0.1	3.3	76.8	4.3	1.0		0.5	0.3		0.01	0.2	0.02	0.05		0.01	0.01
	60		11.9	1.2		0.2	2.6	75.2	6.9	0.9		0.5	0.3		0.01	0.2	0.02	0.06		0.01	<0.01
	61		13.1	1.3		0.1	2.4	72.1	9.0	0.9		0.5	0.3		0.01	0.2	0.02	0.06		0.01	<0.01
	62		12.2	1.1		0.08	2.5	75.2	6.9	0.9		0.5	0.3		0.02	0.2	0.02	0.06		0.01	0.01
	63		12.0	1.00		0.07	2.7	75.5	6.4	1.0		0.6	0.4		0.02	0.2	0.02	0.09		<0.01	<0.01
	64		12.5	1.2		0.1	2.7	75.3	6.2	0.9		0.5	0.3		0.01	0.2	0.02	0.06		0.01	<0.01
	65		13.0	1.1		0.2	2.3	74.5	7.1	0.8		0.4	0.3		0.01	0.2	0.01	0.07		0.01	<0.01
	66		13.3	1.2		0.2	2.3	74.0	7.2	0.8		0.4	0.3		0.01	0.2	0.02	0.06		0.01	<0.01
67		10.7	1.0		0.1	2.7	77.6	5.7	0.9		0.6	0.4		0.02	0.2	0.02	0.05		0.01	<0.01	
Olive/Sunflower	1%		11.1	0.9		0.07	2.8	68.6	13.8	1.4		0.6	0.4		<0.01	0.3	0.01	0.02		<0.01	<0.01
	2%		11.0	1.2		0.1	3.1	67.8	14.1	1.3		0.5	0.5		0.01	0.3	0.02	0.07		<0.01	<0.01
	5%		11.0	1.0		0.2	3.3	63.6	18.1	1.3		0.5	0.5		0.03	0.3	0.07	0.1		<0.01	<0.01
	10%		10.2	0.9		0.1	3.3	61.6	21.0	1.1		0.5	0.7		0.03	0.4	0.06	0.1		0.01	<0.01

Table S4. Number of identified triacylglycerols (TGs) and fatty acids (FAs), average equivalent carbon number (aECN), average carbon number (aCN), average double bond number (aDB), the relative weight concentration [%] of essential fatty acids (linoleic and linolenic acids), fatty acids with eighteen (C18) and sixteen (C16) carbon atoms, saturated (Sat), monounsaturated (Mono) and polyunsaturated (Poly) fatty acids in soya, rapeseed, sunflower and olive cooking oils and in four samples of adulterated olive oil by 1, 2, 5, or 10% of sunflower oil (Olive/Sunflower) calculated from HPLC/APCI-MS of triacylglycerols

Oil	No.	No. of TGs/FAs	aECN	aCN	aDB	Essential FAs [%]	C18+ C16 [%]	Sat [%]	Mono [%]	Poly [%]
Soya	38	66/14	14.86	17.79	1.47	57.0	98.6	16.6	26.4	57.0
	39	66/14	14.80	17.79	1.50	58.5	98.6	16.1	25.4	58.5
Rapeseed	41	55/13	15.29	17.90	1.31	30.9	97.9	9.5	59.6	30.9
	42	55/13	15.30	17.90	1.30	31.0	97.9	9.8	59.2	31.0
Sunflower	44	50/16	14.91	17.88	1.49	61.9	98.1	13.3	24.8	61.9
	45	50/16	14.85	17.88	1.52	64.9	98.2	12.7	22.4	64.9
	46	50/16	14.88	17.87	1.49	63.0	98.1	13.2	23.8	63.0
	47	50/16	14.90	17.86	1.48	61.7	98.2	13.5	24.8	61.7
	48	50/16	14.89	17.87	1.49	62.1	98.1	12.8	25.2	62.1
	49	50/16	14.85	17.88	1.51	64.4	98.2	12.8	22.8	64.4
	50	50/16	14.87	17.88	1.50	63.7	98.2	12.9	23.4	63.7
Olive	51	50/16	14.93	17.87	1.47	61.4	98.1	13.9	24.8	61.4
	53	37/15	15.90	17.75	0.92	7.5	98.5	15.9	76.6	7.5
	54	37/15	15.96	17.75	0.89	5.3	98.8	16.2	78.5	5.3
	55	37/15	15.86	17.72	0.93	9.6	98.9	16.7	73.7	9.6
	56	37/15	15.86	17.76	0.95	9.9	98.6	15.3	74.8	9.9
	57	37/15	15.96	17.75	0.90	5.3	98.8	15.8	78.9	5.3
	58	37/15	15.86	17.71	0.92	9.7	98.8	17.6	72.7	9.7
	59	37/15	15.96	17.74	0.90	5.3	98.8	16.3	78.4	5.3
	60	37/15	15.89	17.75	0.93	7.8	98.7	15.3	76.9	7.8
	61	37/15	15.85	17.72	0.94	9.9	98.8	16.3	73.8	9.9
	62	37/15	15.90	17.75	0.93	7.8	98.8	15.5	76.7	7.8
	63	37/15	15.92	17.76	0.92	7.4	98.6	15.6	77.0	7.4
	64	37/15	15.91	17.74	0.91	7.1	98.8	16.0	76.9	7.1
	65	37/15	15.88	17.72	0.92	7.9	98.8	16.0	76.1	7.9
66	37/15	15.88	17.71	0.92	8.0	98.8	16.3	75.7	8.0	
67	37/15	15.93	17.78	0.93	6.6	98.6	14.3	79.1	6.6	
Olive/Sunflower	1%	37/15	15.75	17.77	1.01	15.2	98.6	14.8	70.0	15.2
	2%	37/15	15.75	17.78	1.01	15.4	98.5	15.0	69.6	15.4
	5%	37/15	15.68	17.78	1.05	19.4	98.3	15.3	65.3	19.4
	10%	37/15	15.65	17.81	1.08	22.1	98.1	14.6	63.3	22.1