Journal of the Serbian Chemical Society
JSCS@tmf.bg.ac.rs • www.shd.org.rs/JSCS

J. Serb. Chem. Soc. 75 (6) S1–S6 (2010)
JSCS–4008

UDC 665.12+641.3:543.544.3+543.51:66.061
Supplementary material

SUPPLEMENTARY MATERIAL TO

Determination of *trans* fatty acids in foodstuffs by gas chromatography–mass spectrometry after simultaneous microwave-assisted extraction–esterification

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J. Serb. Chem. Soc. 75 (6) (2010) 803–812

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TABLE I. Saturated fatty acids composition, as % of total fatty acids, of foodstuffs obtained by Soxhlet, MAE and SMAEE methods (values are the means of three determinations±standard deviation; the shorthand names of the fatty acid are given in the form: number of carbon atoms in the molecule followed by the number of double bonds; the two number are separated by a colon)

Sample	Method	Fatty acid					
		6:0	8:0	10:0	12:0	14:0	15:0
Caramel	SE[a]	0.87±0.07	3.62±0.13	3.96±0.05	27.19±0.00	12.60±0.19	0.61±0.03
	MAE[b]	0.96±0.05	3.77±0.19	3.95±0.09	28.46±0.24	12.61±0.15	0.46±0.03
	SMAEE[c]	1.15±0.04	4.03±0.20	3.87±0.07	28.91±0.11	12.76±0.18	0.53±0.05
Cracker 1	SE	–	1.65±0.11	1.17±0.01	8.11±0.36	2.85±0.06	–
	MAE	–	1.15±0.10	0.80±0.03	6.62±0.26	2.61±0.09	–
	SMAEE	–	0.89±0.02	0.66±0.03	6.82±0.14	2.35±0.03	–
Biscuit	SE	–	2.65±0.12	3.42±0.03	9.14±0.20	10.05±0.10	0.93±0.07
	MAE	–	2.68±0.09	3.33±0.07	8.72±0.21	9.66±0.50	0.94±0.02
	SMAEE	–	2.60±0.05	3.50±0.04	8.76±0.19	9.81±0.23	1.04±0.02
Cookie 1	SE	–	3.00±0.03	2.13±0.09	13.76±0.23	5.65±0.01	–
	MAE	–	3.38±0.11	2.21±0.03	13.01±0.45	5.58±0.03	–
	SMAEE	–	3.73±0.12	2.31±0.02	13.56±0.54	5.58±0.03	–
Cookie 2	SE	–	2.16±0.14	1.49±0.06	10.17±0.15	4.33±0.28	–
	MAE	–	2.65±0.18	1.75±0.10	10.45±0.12	4.31±0.06	–
	SMAEE	–	2.31±0.11	1.60±0.03	10.06±0.11	4.22±0.02	–
Cracker 2	SE	–	3.21±0.00	2.41±0.11	14.09±0.15	5.27±0.10	–
	MAE	–	3.84±0.05	2.60±0.12	14.25±0.21	5.16±0.08	–
	SMAEE	–	3.40±0.07	2.60±0.17	14.05±0.29	4.64±0.06	–
Milk chocolate	SE	–	1.97±0.01	1.52±0.04	8.98±0.02	4.39±0.11	–
	MAE	0.22±0.01	1.83±0.05	1.43±0.06	7.52±0.06	3.97±0.13	0.12±0.01
	SMAEE	0.28±0.02	2.21±0.01	1.68±0.03	8.84±0.14	4.46±0.14	0.16±0.00
Croissant with cocoa	SE	–	–	–	0.56±0.02	1.37±0.05	–
	MAE	–	–	–	0.52±0.01	1.40±0.02	–
	SMAEE	–	–	–	0.53±0.00	1.29±0.07	–

TABLE I. Continued

Sample	Method	Fatty acid					
		6:0	8:0	10:0	12:0	14:0	15:0
Chocolate with coconut	SE	–	9.32±0.41	5.20±0.46	29.25±1.17	9.05±0.33	–
	MAE	–	9.64±0.10	5.26±0.48	30.09±1.80	9.18±0.21	–
	SMAEE	–	9.17±0.50	5.34±0.04	30.77±1.76	9.16±0.28	–
Chocolate with rice	SE	–	–	–	0.33±0.03	0.91±0.06	–
	MAE	–	–	0.41±0.04	0.46±0.02	1.11±0.02	–
	SMAEE	–	–	0.71±0.04	0.67±0.01	1.77±0.02	–
Cookie 3	SE	–	1.71±0.04	1.60±0.01	17.67±0.07	5.96±0.11	–
	MAE	–	1.88±0.01	1.53±0.02	17.01±0.08	5.66±0.10	–
	SMAEE	–	1.92±0.01	1.70±0.02	17.21±0.07	5.92±0.08	–
		16:0	17:0	18:0	20:0	22:0	
Caramel	SE	17.56±0.14	0.40±0.04	15.86±0.30	0.23±0.01	–	
	MAE	17.48±0.00	0.34±0.04	15.94±0.20	0.26±0.02	–	
	SMAEE	17.56±0.19	0.34±0.03	15.19±0.29	0.19±0.00	–	
Cracker 1	SE	19.50±0.32	–	7.38±0.10	0.44±0.02	0.36±0.04	
	MAE	18.26±0.23	–	7.52±0.12	0.36±0.02	0.36±0.01	
	SMAEE	18.91±0.25	–	7.73±0.14	0.40±0.03	0.39±0.01	
Biscuit	SE	32.48±0.36	0.58±0.02	7.38±0.04	–	–	
	MAE	32.13±0.16	0.59±0.03	7.44±0.08	0.24±0.02	–	
	SMAEE	32.03±0.25	0.54±0.03	8.05±0.04	0.20±0.02	–	
Cookie 1	SE	31.77±0.02	–	5.19±0.03	0.31±0.03	–	
	MAE	31.59±0.11	–	5.19±0.05	0.32±0.02	–	
	SMAEE	31.31±0.16	–	4.92±0.07	0.32±0.01	–	
Cookie 2	SE	25.61±0.14	–	4.09±0.01	0.23±0.02	–	
	MAE	26.22±0.09	–	4.12±0.03	0.26±0.01	–	
	SMAEE	26.56±0.10	–	4.22±0.03	0.27±0.02	–	

TABLE I. Continued

Sample	Method	Fatty acid				
		16:0	17:0	18:0	20:0	22:0
Cracker 2	SE	31.68±0.03	–	3.73±0.01	0.30±0.01	–
	MAE	31.22±0.25	–	3.66±0.16	0.27±0.03	–
	SMAEE	31.95±0.39	–	3.71±0.15	0.22±0.03	–
Milk chocolate	SE	30.48±0.11	–	17.82±0.12	0.61±0.03	–
	MAE	29.92±0.39	0.25±0.01	19.52±0.14	0.66±0.06	0.15±0.01
	SMAEE	29.86±0.04	0.23±0.00	18.34±0.24	0.58±0.05	0.08±0.00
Croissant with cocoa	SE	45.13±0.84	0.17±0.02	5.35±0.20	0.40±0.03	0.11±0.01
	MAE	43.20±0.11	0.13±0.00	6.47±0.00	0.45±0.03	0.11±0.01
	SMAEE	43.14±0.24	0.14±0.00	6.53±0.10	0.39±0.03	0.13±0.00
Chocolate with coconut	SE	14.20±0.87	–	16.62±0.82	0.55±0.05	–
	MAE	14.42±1.30	–	14.39±0.98	0.56±0.01	–
	SMAEE	14.29±0.35	–	14.07±0.82	0.52±0.00	–
Chocolate with rice	SE	15.76±1.19	–	10.61±0.21	0.48±0.04	0.28±0.01
	MAE	17.58±0.15	–	9.72±0.15	0.40±0.00	0.21±0.00
	SMAEE	18.68±0.35	–	9.85±0.06	0.41±0.02	0.18±0.02
Cookie 3	SE	30.68±0.91	–	4.28±0.21	0.32±0.02	–
	MAE	30.68±0.95	–	4.11±0.17	0.30±0.03	–
	SMAEE	30.55±0.87	–	4.32±0.14	0.27±0.03	–

[a]Soxhlet extraction; [b]microwave-assisted extraction; [c]microwave-assisted extraction–esterification

TABLE II. Unaturated fatty acids composition, as % of total fatty acids, of foodstuffs obtained by Soxhlet, MAE and SMAEE methods (values are the means of three determinations±standard deviation; the shorthand names of the fatty acid are given in the form: number of carbon atoms in the molecule followed by the number of double bonds and indication of structural configuration; the two number are separated by a colon)

Sample	Method	Fatty acid							
		14:1	16:1	18:1 *trans*	18:1 *cis*	18:2 *trans*	18:2 *cis*	20:1	18:3
Caramel	SE[a]	0.40±0.00	0.79±0.00	1.88±0.02	9.92±0.26	–	3.82±0.02	–	0.29±0.01
	MAE[b]	0.40±0.02	0.69±0.04	1.77±0.02	9.23±0.03	–	3.46±0.02	–	0.22±0.01
	SMAEE[c]	0.35±0.02	0.74±0.04	1.84±0.03	8.59±0.12	–	3.71±0.09	–	0.24±0.00
Cracker 1	SE	–	–	18.36±0.08	29.59±0.71	1.70±0.12	8.89±0.13	–	–
	MAE	–	–	18.26±0.18	31.22±0.01	1.80±0.04	10.74±0.15	0.15±0.01	0.15±0.01
	SMAEE	–	–	18.22±0.15	31.39±0.27	1.85±0.07	10.03±0.05	0.15±0.01	0.21±0.02
Biscuit	SE	0.63±0.05	1.33±0.10	1.19±0.08	22.37±0.11	–	7.42±0.01	–	0.43±0.04
	MAE	0.67±0.00	1.42±0.08	1.24±0.04	22.74±0.78	–	7.75±0.18	–	0.45±0.02
	SMAEE	0.67±0.01	1.25±0.06	1.09±0.07	21.64±0.39	–	8.39±0.17	–	0.43±0.03
Cookie 1	SE	–	–	0.46±0.03	29.05±0.32	–	8.68±0.06	–	–
	MAE	–	–	0.33±0.02	29.57±0.51	–	8.66±0.16	–	0.16±0.01
	SMAEE	–	–	0.34±0.01	28.74±0.41	–	8.98±0.12	–	0.21±0.02
Cookie 2	SE	–	–	–	40.53±0.16	–	11.39±0.05	–	–
	MAE	–	0.13±0.01	–	38.61±0.77	–	11.10±0.03	0.17±0.01	0.23±0.02
	SMAEE	–	0.16±0.01	–	38.46±0.16	–	11.66±0.04	0.22±0.02	0.26±0.02
Cracker 2	SE	–	–	–	25.64±0.13	–	13.67±0.19	–	–
	MAE	–	–	–	25.10±0.25	–	13.90±0.57	–	–
	SMAEE	–	–	–	25.90±0.88	–	13.53±0.43	–	–
Milk chocolate	SE	–	0.22±0.00	–	27.91±0.05	–	6.10±0.01	–	–
	MAE	–	0.29±0.01	–	28.34±0.06	–	5.63±0.11	–	0.15±0.01
	SMAEE	–	0.28±0.00	–	26.82±0.06	–	5.98±0.05	–	0.20±0.01
Croissant with cocoa	SE	–	0.17±0.05	2.15±0.10	31.97±0.54	–	12.28±0.24	0.15±0.02	0.19±0.02
	MAE	–	0.12±0.00	2.13±0.02	31.81±0.02	–	13.34±0.06	0.13±0.02	0.19±0.02
	SMAEE	–	0.11±0.00	2.00±0.03	31.05±0.03	–	14.33±0.12	0.14±0.00	0.22±0.02

TABLE II. Continued

Sample	Method	Fatty acid							
		14:1	16:1	18:1 *trans*	18:1 *cis*	18:2 *trans*	18:2 *cis*	20:1	18:3
Chocolate with coconut	SE[a]	–	–	1.05±0.08	13.70±1.36	–	1.06±0.19	–	–
	MAE[b]	–	–	1.16±0.11	14.30±0.94	–	1.00±0.13	–	–
	SMAEE[c]	–	–	1.10±0.11	14.44±1.08	–	1.14±0.13	–	–
Chocolate with rice	SE	–	–	41.65±0.89	29.31±1.48	–	0.67±0.02	–	–
	MAE	–	–	36.31±0.65	32.28±0.08	–	1.52±0.09	–	–
	SMAEE	–	–	34.94±0.66	31.03±1.04	–	1.76±0.07	–	–
Cookie 3	SE	–	–		28.04±1.03	–	9.74±0.07	–	–
	MAE	–	–		28.72±0.46	–	10.11±0.08	–	–
	SMAEE	–	–		28.36±0.37	–	9.75±0.07	–	–

[a]Soxhlet extraction; [b]microwave-assisted extraction; [c]microwave-assisted extraction–esterification