

Supplementary Information

Ultrasonic Extracts of *Morinda citrifolia* L.: Characterization of Volatile Compounds by Gas Chromatography-Mass Spectrometry

Daiane B. M. Lima,^a Anaí L. dos Santos,^b Ariel O. Celestino,^a Nayna Sampaio,^a Jéssica Baldez,^a Maria I. S. Melecchi,^c Thiago R. Bjerk,^a Laíza C. Krause^{a,d} and Elina B. Caramão^{,a,b,d}*

^a*Programa de Pós-Graduação em Biotecnologia Industrial (PBI), Universidade Tiradentes (UNIT), Av. Murilo Dantas, 300, 49032-490 Aracaju-SE, Brazil*

^b*Programa de Pós-Graduação em Química (PPGQ), Universidade Federal do Rio Grande do Sul (UFRGS), Av. Bento Gonçalves, 9500, 90040-060 Porto Alegre-RS, Brazil*

^c*Colégio Militar de Porto Alegre (CMPA), Av. José Bonifácio, 363, Farroupilha, 90040-130 Porto Alegre-RS, Brazil*

^d*Instituto Nacional Ciência e Tecnologia em Energia e Ambiente (INCT E&A), Universidade Federal da Bahia (UFBA), 40170-110 Salvador-BA, Brazil*

*e-mail: elina@ufrgs.br

Statistical treatments

In Figure S1 it is represented the response surface graph. The analysis of Figure S1 shows that in (A) the optimum yield is obtained when using the higher temperature and longer extraction time (55 °C and 150 min), while in (B) the higher yield occurs in lower masses and higher temperatures (1 g and 55 °C). In (C), the best value is assigned to lower mass and longer time (1 g and 150 min).

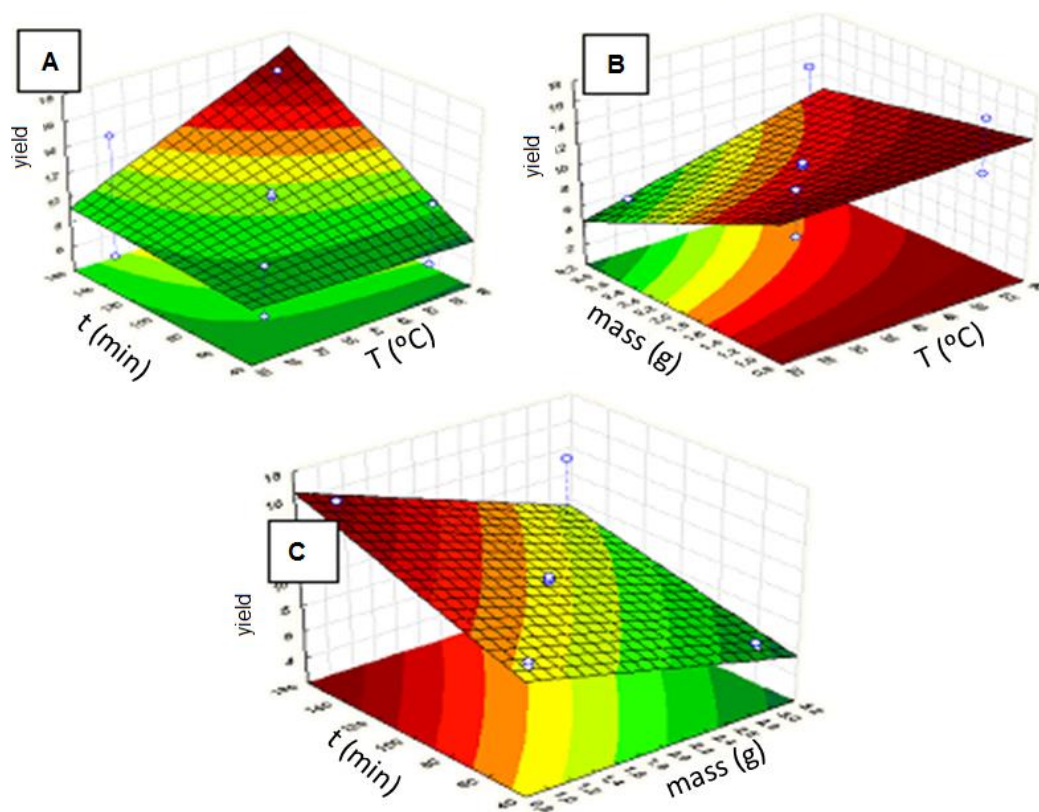


Figure S1. Response surfaces for: (A) temperature (°C) and time (min) in the extractive process; (B) mass (g) and temperature (°C); and (C) time (min) and mass (g).

Peak identification of extracts by GC-MS

Tables S1 and S2 show the peak identification of compounds according to Figure 3 in the manuscript.

Table S1. Identification of the compounds of leaves extracts of *M. citrifolia* L., according to Figure 3

Class	Peak	t _R / min	Name	Formula	Comp. / %		LTPRI			Identification
					Hexane	Ethanol	Experimental	NIST	Difference	
Acid	1	22.79	octanoic acid	C ₈ H ₁₆ O ₂	n.d.	0.87	1168	1169	-2	LTPRI, MS
Acid	23	71.66	hexadecanoic acid	C ₁₈ H ₃₆ O ₂	n.d.	2.40	1961	1968	-8	LTPRI, MS
Acid	31	80.76	linoleic acid	C ₁₈ H ₃₀ O ₂	3.56	5.56	2150	2154	-5	LTPRI, MS
Acid	32	81.49	9,12-octadecenoic acid (Z,Z)	C ₁₈ H ₃₂ O ₂	n.d.	0.76	2166	2170	-6	LTPRI, MS
Acid	34	81.84	9-octadecenoic acid	C ₁₈ H ₃₆ O ₂	n.d.	4.47	2174	2175	-3	LTPRI, MS
Alcohol	17	65.41	8-hexadecenol, Z	C ₁₆ H ₃₂ O	0.54	8.22	1846	1862	-17	LTPRI, MS
Alcohol	19	66.72	10-hexadecenol, E	C ₁₆ H ₃₀ O	n.d.	0.93	1869	1869	-2	LTPRI, MS
Alcohol	20	67.69	14-hexadecenol, E	C ₁₆ H ₃₀ O	n.d.	2.73	1886	1887	-3	LTPRI, MS
Alcohol	26	77.76	1-octadecanol	C ₁₈ H ₃₆ O	n.d.	0.11	2086	2081	4	LTPRI, MS
Alcohol	30	79.29	cis-phytol	C ₂₀ H ₄₀ O	2.51	6.93	2118	2119	-2	LTPRI, MS
Alcohol	48	107.03	1-pentacosanol	C ₂₅ H ₅₂ O	n.d.	0.07	2797	n.f.	n.f.	MS
Alcohol	56	114.25	1-heptacosanol	C ₂₇ H ₅₆ O	1.70	0.08	2998	3016	-19	LTPRI, MS
Alcohol	61	119.57	1-octacosanol	C ₂₈ H ₅₈ O	n.d.	0.05	3127	3120	6	LTPRI, MS
Aldehyde	4	27.30	5-hydroxymethylfurfural	C ₆ H ₆ O ₃	n.d.	8.08	1234	1232	1	LTPRI, MS
Aldehyde	38	88.78	heneicosanal	C ₂₁ H ₄₂ O	n.d.	0.10	2331	2332	-3	LTPRI, MS
Aldehyde	40	97.16	tricosanal	C ₂₃ H ₄₆ O	n.d.	0.04	2534	2532	1	LTPRI, MS
Aldehyde	66	131.91	tritriacontanal	C ₃₃ H ₆₆ O	n.d.	0.08	3358	n.f.	n.f.	MS

Table S1. Identification of the compounds of leaves extracts of *M. citrifolia* L., according to Figure 3 (cont.)

Class	Peak	t _R / min	Name	Formula	Comp. / %			LTPRI		Identification
					Hexane	Ethanol	Experimental	NIST	Difference	
Aldehyde	67	139.20	tetratriacontanal	C ₃₄ H ₆₈ O	n.d.	0.53	3491	n.f.	n.f.	MS
Aldehyde	68	141.39	pentatriacontanal	C ₃₅ H ₇₀ O	n.d.	0.67	3531	n.f.	n.f.	MS
Aldehyde	69	145.17	hexatriacontanal	C ₃₆ H ₇₂ O	n.d.	0.51	3599	n.f.	n.f.	MS
Ester	3	24.73	ethyl octanoate	C ₁₀ H ₂₂ O ₂	n.d.	1.26	1197	1197	-1	LTPRI, MS
Ester	11	38.48	ethyl decanoate	C ₁₂ H ₂₆ O ₂	n.d.	3.26	1396	1396	-1	LTPRI, MS
Ester	13	51.30	ethyl dodecanoate	C ₁₄ H ₃₀ O ₂	n.d.	1.04	1594	1593	-1	LTPRI, MS
Ester	22	69.89	methyl hexadecanoate	C ₁₇ H ₃₆ O ₂	n.d.	0.19	1927	1927	-2	LTPRI, MS
Ester	24	73.32	methyl hexadecenoate	C ₁₇ H ₃₄ O ₂	0.62	1.04	1994	1994	-1	LTPRI, MS
Ester	27	78.36	methyl 9,12-octadecenoate	C ₁₉ H ₃₄ O ₂	n.d.	0.31	2099	2092	6	LTPRI, MS
Ester	29	78.71	methyl elaidate	C ₁₉ H ₃₂ O ₂	0.85	1.01	2106	2108	-3	LTPRI, MS
Ester	33	81.51	ethyl linoleate	C ₂₀ H ₃₆ O ₂	1.61	n.d.	2166	2163	2	LTPRI, MS
Ester	35	81.86	ethyl elaidate	C ₂₀ H ₃₄ O ₂	3.96	n.d.	2174	2173	0	LTPRI, MS
Ester	36	82.82	ethyl stearate	C ₂₀ H ₄₀ O ₂	n.d.	0.17	2194	2194	-1	LTPRI, MS
Hc	5	30.61	2,6,11-trimethyldodecane	C ₁₅ H ₃₂	0.08	n.d.	1282	1275	6	LTPRI, MS
Hc	7	33.79	4,6-dimethyldodecane	C ₁₄ H ₃₀	0.10	n.d.	1328	1325	2	LTPRI, MS
Hc	8	34.46	3-ethyl, 3-methyl undecane	C ₁₄ H ₃₀	0.04	n.d.	1337	1347	-11	LTPRI, MS
Hc	9	36.66	1,1,4,5-tetramethyl indane	C ₁₃ H ₁₈	0.08	n.d.	1362	1355	6	LTPRI, MS
Hc	12	39.98	2,6-dimethyl-naphthalene	C ₁₂ H ₁₃	0.03	n.d.	1418	1416	1	LTPRI, MS
Hc	14	57.57	<i>n</i> -heptadecane	C ₁₇ H ₃₆	0.04	n.d.	1700	1700	-1	LTPRI, MS
Hc	16	65.13	2-phytene	C ₂₀ H ₄₀	n.d.	0.17	1841	1833	7	LTPRI, MS
Hc	18	65.76	1-phytene	C ₂₀ H ₄₀	0.05	0.42	1852	1849	2	LTPRI, MS
Hc	21	68.53	<i>n</i> -nonadecane	C ₂₁ H ₄₄	0.12	n.d.	1900	1900	-1	LTPRI, MS
Hc	25	73.61	<i>n</i> -eicosane	C ₂₀ H ₄₂	0.24	n.d.	2000	2000	-1	LTPRI, MS
Hc	28	78.44	<i>n</i> -heneicosane	C ₂₁ H ₄₄	0.47	n.d.	2100	2100	-1	LTPRI, MS
Hc	37	87.49	<i>n</i> -tricosane	C ₂₃ H ₄₈	0.23	n.d.	2300	2300	-1	LTPRI, MS

Table S1. Identification of the compounds of leaves extracts of *M. citrifolia* L., according to Figure 3 (cont.)

Class	Peak	t _R / min	Name	Formula	Comp. / %			LTPRI		Identification
					Hexane	Ethanol	Experimental	NIST	Difference	
Hc	39	95.79	<i>n</i> -pentacosane	C ₂₅ H ₅₂	1.68	0.18	2500	2500	-1	LTPRI, MS
Hc	41	97.18	2-methylpentacosane	C ₂₆ H ₅₄	0.15	n.d.	2535	2533	1	LTPRI, MS
Hc	42	99.67	hexacosane	C ₂₆ H ₅₄	1.48	0.15	2600	2600	-1	LTPRI, MS
Hc	43	101.02	12-methyl-hexacosane	C ₂₇ H ₅₆	1.53	n.d.	2634	2631	2	LTPRI, MS
Hc	44	101.99	2-methyl-hexacosane	C ₂₇ H ₅₆	3.55	n.d.	2660	2663	-4	LTPRI, MS
Hc	45	102.97	3-methyl-hexacosane	C ₂₇ H ₅₆	1.63	n.d.	2686	2672	13	LTPRI, MS
Hc	46	103.49	<i>n</i> -heptacosane	C ₂₇ H ₅₆	0.24	0.28	2700	2700	-1	LTPRI, MS
Hc	47	104.72	13-methyl-heptacosane	C ₂₈ H ₅₈	2.86	n.d.	2734	2731	2	LTPRI, MS
Hc	49	107.15	<i>n</i> -octacosane	C ₂₈ H ₅₈	1.63	0.14	2801	2800	0	LTPRI, MS
Hc	50	108.34	14-methyl-octacosane	C ₂₉ H ₆₀	2.05	n.d.	2834	2829	4	LTPRI, MS
Hc	51	108.62	squalene	C ₃₀ H ₅₀	12.72	30.05	2844	2847	-4	LTPRI, MS
Hc	52	110.66	<i>n</i> -nonacosane	C ₂₉ H ₆₀	6.43	2.33	2901	2900	0	LTPRI, MS
Hc	53	111.40	15-methyl-nonacosane	C ₃₀ H ₆₂	0.54	n.d.	2921	2929	-9	LTPRI, MS
Hc	54	111.80	11-methyl-nonacosane	C ₃₀ H ₆₂	3.00	n.d.	2931	2932	-2	LTPRI, MS
Hc	55	113.39	13-methyl-nonacosane	C ₃₀ H ₆₂	2.84	n.d.	2974	2972	1	LTPRI, MS
Hc	57	114.36	<i>n</i> -triacontane	C ₃₀ H ₆₂	3.11	0.67	3001	3000	0	LTPRI, MS
Hc	58	115.60	4-methyl-triacontane	C ₃₁ H ₆₄	5.59	n.d.	3031	3035	-5	LTPRI, MS
Hc	59	116.94	2-methyl-triacontane	C ₃₁ H ₆₄	2.87	n.d.	3063	3060	2	LTPRI, MS
Hc	60	118.55	<i>n</i> -hentriacontane	C ₃₁ H ₆₄	9.82	7.64	3103	3100	2	LTPRI, MS
Hc	62	119.89	3-methyl-hentriacontane	C ₃₂ H ₆₆	3.52	n.d.	3130	3132	-3	LTPRI, MS
Hc	64	124.80	14-methyl-dotriacontane	C ₃₃ H ₆₈	2.65	n.d.	3229	3230	-2	LTPRI, MS
Hc	65	130.58	13-methyl-tritriacontane	C ₃₃ H ₆₈	1.69	n.d.	3334	3332	1	LTPRI, MS
Ketone	15	58.50	4-(3-hydroxybutyl)-3,5,5-trimethyl-2-cyclohexen-1-one	C ₁₃ H ₂₂ O ₂	0.18	n.d.	1718	1713	4	LTPRI, MS
Phenol	2	23.25	4-methyl-guaiacol	C ₈ H ₁₀ O ₂	n.d.	0.27	1175	1181	-7	LTPRI, MS
Phenol	6	33.39	4-vinyl-guaiacol	C ₉ H ₁₀ O ₂	n.d.	0.58	1322	1321	0	LTPRI, MS

Table S1. Identification of the compounds of leaves extracts of *M. citrifolia* L., according to Figure 3 (cont.)

Class	Peak	t _R / min	Name	Formula	Comp. / %			LTPRI		Identification
					Hexane	Ethanol	Experimental	NIST	Difference	
Phenol	10	37.04	4-propyl-guaiacol	C ₁₀ H ₁₄ O ₂	n.d.	0.17	1375	1375	-1	LTPRI, MS
Vit	63	121.38	α-tocopherol (vitamin E)	C ₂₉ H ₅₀ O ₂	11.41	5.51	3163	3150	12	LTPRI, MS

Comp.: composition (in percentage) obtained by the direct comparison between the areas of the peaks identified; LTPRI: linear temperature programmed retention indexes; MS: mass spectrometry; n.d.: not detected; n.f.: LTPRI not found in the literature; Hc: hydrocarbon; Vit: vitamin.

Table S2. Identification of the compounds of fruit extracts of *M. citrifolia* L., according to Figure 3

Class	Peak	t _R / min	Name	Formula	Area / %			LTPRI		Identification
					Hexane	Ethanol	Experimental	NIST	Difference	
Acid	1	11.61	2-methyl pentanoic acid	C ₆ H ₁₂ O ₂	n.d.	3.01	998	984	14	LTPRI, MS
Acid	2	11.92	hexanoic acid	C ₆ H ₁₂ O ₂	n.d.	9.44	1003	1008	-5	LTPRI, MS
Acid	3	22.81	octanoic acid	C ₈ H ₁₆ O ₂	0.25	25.58	1180	1178	2	LTPRI, MS
Acid	6	36.32	decanoic acid	C ₁₀ H ₂₀ O ₂	n.d.	0.51	1364	1360	4	LTPRI, MS
Acid	13	71.76	hexadecanoic acid	C ₁₆ H ₃₂ O ₂	0.38	1.76	1964	1963	1	LTPRI, MS
Acid	22	81.50	9,12-octadecenoic acid	C ₁₈ H ₃₄ O ₂	n.d.	2.59	2166	2163	3	LTPRI, MS
Alcohol	21	80.99	1-nonadecanol	C ₁₉ H ₄₀ O	n.d.	0.71	2143	2156	-13	LTPRI, MS
Alcohol	60	127.31	gamma-sitosterol	C ₂₉ H ₅₀ O	n.d.	0.99	3275	3290	-15	LTPRI, MS
Aldehyde	5	27.19	5-hydroxymethylfurfural	C ₆ H ₆ O ₃	n.d.	14.28	1233	1233	0	LTPRI, MS
Aldehyde	30	87.45	nonadecanal	C ₁₉ H ₃₈ O	n.d.	1.69	2299	2329	-30	MS
Aldehyde	33	92.91	docosanal	C ₂₂ H ₄₄ O	n.d.	0.62	2429	2431	-2	LTPRI, MS
Ester	4	24.76	ethyl-octanoate	C ₁₀ H ₂₀ O ₂	n.d.	1.82	1198	1198	0	LTPRI, MS
Ester	8	38.48	ethyl decanoate	C ₁₂ H ₂₄ O ₂	n.d.	2.32	1395	1391	4	LTPRI, MS
Ester	9	41.91	3-methylbutyl octanoate	C ₁₃ H ₂₆ O ₂	n.d.	0.85	1447	1450	-3	LTPRI, MS
Ester	10	51.32	methyl pentadecanoate	C ₁₆ H ₃₂ O ₂	n.d.	1.19	1594	1593	1	LTPRI, MS

Table S2. Identification of the compounds of fruit extracts of *M. citrifolia* L., according to Figure 3 (cont.)

Class	Peak	t _R / min	Name	Formula	Area / %		LTPRI			Identification
					Hexane	Ethanol	Experimental	NIST	Difference	
Ester	12	69.91	methyl hexadecanoate	C ₁₇ H ₃₄ O ₂	0.16	2.62	1927	1926	1	LTPRI, MS
Ester	15	73.34	methyl hexadecenoate	C ₁₇ H ₃₄ O ₂	0.35	2.88	1995	1994	1	LTPRI, MS
Ester	17	78.38	methyl-9,12-octadecenoate	C ₁₉ H ₃₆ O ₂	n.d.	0.67	2098	2092	6	LTPRI, MS
Ester	19	78.62	methyl elaidate	C ₁₉ H ₃₂ O ₂	n.d.	0.63	2104	2103	1	LTPRI, MS
Ester	20	79.77	methyl stearate	C ₁₉ H ₃₈ O ₂	0.19	0.60	2128	2128	0	LTPRI, MS
Ester	23	81.53	ethyl linoleate	C ₁₉ H ₃₄ O ₂	0.26	n.d.	2167	2163	4	LTPRI, MS
Ester	24	81.75	ethyl oleate	C ₂₀ H ₃₈ O ₂	0.45	4.37	2172	2171	1	LTPRI, MS
Ester	25	82.00	ethyl elaidate	C ₂₀ H ₃₈ O ₂	n.d.	1.32	2174	2174	0	LTPRI, MS
Ester	26	82.83	ethyl stearate	C ₂₀ H ₄₀ O ₂	n.d.	0.77	2195	2195	0	LTPRI, MS
Ester	29	85.16	3-methylbutyl hexadecanoate	C ₂₁ H ₄₂ O ₂	n.d.	0.63	2247	2246	1	LTPRI, MS
Hc	11	68.55	<i>n</i> -nonadecane	C ₁₉ H ₄₀	0.13	n.d.	1900	1900	0	LTPRI, MS
Hc	16	73.63	<i>n</i> -eicosane	C ₂₀ H ₄₂	0.24	n.d.	2000	2000	0	LTPRI, MS
Hc	18	78.47	<i>n</i> -heneicosane	C ₂₁ H ₄₄	0.27	n.d.	2100	2100	0	LTPRI, MS
Hc	27	83.10	<i>n</i> -docosane	C ₂₂ H ₄₆	0.36	n.d.	2201	2200	1	LTPRI, MS
Hc	28	84.77	5-methyl-docosane	C ₂₃ H ₄₈	0.33	n.d.	2238	2252	-14	LTPRI, MS
Hc	31	87.53	<i>n</i> -tricosane	C ₂₃ H ₄₈	0.31	n.d.	2301	2300	1	LTPRI, MS
Hc	32	91.73	<i>n</i> -tetracosane	C ₂₄ H ₅₀	n.d.	0.59	2400	2400	0	LTPRI, MS
Hc	34	95.83	<i>n</i> -pentacosane	C ₂₅ H ₅₂	2.03	1.75	2501	2500	1	LTPRI, MS
Hc	35	96.17	5-ethyl-5-methyl-tricosane	C ₁₃ H ₂₈	1.15	n.d.	2509	2515	-6	LTPRI, MS
Hc	36	97.24	13-methyl-pentacosane	C ₂₆ H ₅₄	2.08	n.d.	2536	2536	0	LTPRI, MS
Hc	37	99.74	<i>n</i> -hexacosane	C ₂₆ H ₅₄	1.70	0.69	2601	2600	1	LTPRI, MS
Hc	38	101.06	12-methyl-hexacosane	C ₂₆ H ₅₄	2.33	n.d.	2635	2631	4	LTPRI, MS
Hc	39	102.06	2-methyl-hexacosane	C ₂₇ H ₅₆	1.55	n.d.	2662	2662	0	LTPRI, MS
Hc	40	103.52	<i>n</i> -heptacosane	C ₂₇ H ₅₆	1.39	0.66	2702	2700	2	LTPRI, MS

Table S2. Identification of the compounds of fruit extracts of *M. citrifolia* L., according to Figure 3 (cont.)

Class	Peak	t _R / min	Name	Formula	Area / %		LTPRI			Identification
					Hexane	Ethanol	Experimental	NIST	Difference	
Hc	41	104.78	13-methyl-heptacosane	C ₂₈ H ₅₈	2.28	n.d.	2735	2731	4	LTPRI, MS
Hc	42	105.03	7-methyl-heptacosane	C ₂₈ H ₅₈	1.49	n.d.	2742	2741	1	LTPRI, MS
Hc	43	106.27	3-methyl-heptacosane	C ₂₈ H ₅₈	1.05	n.d.	2776	2773	3	LTPRI, MS
Hc	44	107.16	<i>n</i> -octacosane	C ₂₈ H ₅₈	1.36	0.96	2802	2800	2	LTPRI, MS
Hc	45	108.36	14-methyl-octacosane	C ₂₉ H ₆₀	3.06	n.d.	2835	2829	6	LTPRI, MS
Hc	46	108.54	squalene	C ₃₀ H ₅₀	2.39	5.22	2841	2847	-6	LTPRI, MS
Hc	47	110.05	3-methyl-octacosane	C ₂₉ H ₆₀	1.69	n.d.	2883	2873	10	LTPRI, MS
Hc	48	110.68	<i>n</i> -nonacosane	C ₂₉ H ₆₀	4.45	1.74	2902	2900	2	LTPRI, MS
Hc	49	111.48	13-methyl-nonacosane	C ₃₀ H ₆₂	2.89	n.d.	2923	2931	-8	LTPRI, MS
Hc	50	111.87	11-methyl-nonacosane	C ₃₀ H ₆₂	3.52	n.d.	2933	2932	1	LTPRI, MS
Hc	51	113.48	3-methyl-nonacosane	C ₃₀ H ₆₂	3.17	n.d.	2977	2972	5	LTPRI, MS
Hc	52	114.40	<i>n</i> -triacontane	C ₃₀ H ₆₂	2.19	1.39	3003	3000	3	LTPRI, MS
Hc	53	115.72	11-methyl-triacontane	C ₃₁ H ₆₄	6.47	n.d.	3034	3035	-1	LTPRI, MS
Hc	54	117.05	2-methyl-triacontane	C ₃₁ H ₆₄	2.61	n.d.	3066	3061	5	LTPRI, MS
Hc	56	117.81	3-methyl-triacontane	C ₃₁ H ₆₄	3.82	n.d.	3085	3078	7	LTPRI, MS
Hc	57	118.55	<i>n</i> -hentriacontane	C ₃₁ H ₆₄	7.93	1.44	3104	3100	4	LTPRI, MS
Hc	35	96.17	5-ethyl-5-methyl-tricosane	C ₁₃ H ₂₈	1.15	n.d.	2509	2515	-6	LTPRI, MS
Hc	59	125.00	14-methyl-dotriacontane	C ₃₃ H ₆₈	5.36	n.d.	3233	3230	3	LTPRI, MS
Hc	61	130.82	13-methyl-tritriacontane	C ₃₄ H ₇₀	4.36	n.d.	3339	3332	7	LTPRI, MS
Hc	62	132.26	17-methyl-tetratriacontane	C ₃₅ H ₇₂	3.24	n.d.	3421	3423	-2	LTPRI, MS
Hc	63	135.25	4-methyl-tetratriacontane	C ₃₅ H ₇₂	3.73	n.d.	3464	3461	3	LTPRI, MS
Hc	64	140.16	5-methyl-pentatriacontane	C ₃₆ H ₇₄	2.21	n.d.	3563	3553	10	LTPRI, MS
Hc	65	143.90	3-methyl-pentatriacontane	C ₃₆ H ₇₄	2.64	n.d.	3576	3574	2	LTPRI, MS
Hc	66	146.02	<i>n</i> -hexatriacontane	C ₃₆ H ₇₄	1.74	n.d.	3615	3600	15	LTPRI, MS

Table S2. Identification of the compounds of fruit extracts of *M. citrifolia* L., according to Figure 3 (cont.)

Class	Peak	t _R / min	Name	Formula	Area / %		LTPRI			Identification
					Hexane	Ethanol	Experimental	NIST	Difference	
Ketone	14	72.85	scopoletin (7-hydroxy-6-methoxychromen-2-one)	C ₁₀ H ₈ O ₄	n.d.	1.09	1985	n.f.	n.f.	MS
Phenol	7	37.04	4-propyl-guaiacol	C ₁₀ H ₁₄ O ₂	n.d.	0.62	1375	1375	0	LTPRI, MS
Vitamin	55	117.63	gamma-tocopherol	C ₂₈ H ₄₈ O ₂	2.72	n.d.	3080	3055	25	LTPRI, MS
Vitamin	58	121.37	α-tocopherol (vitamin E)	C ₂₉ H ₅₀ O ₂	7.68	2.00	3164	3150	15	LTPRI, MS

Comp.%: Composition (%) obtained by the direct comparison between the areas of the peaks identified (comp.% used instead of area% only for semi-quantitative purposes); LTPRI: linear temperature programmed retention indexes; MS: mass spectrometry; n.d.: not detected; n.f.: LTPRI not found in the literature; Hc: hydrocarbon; Vit: vitamin.

Table S3. Distribution of the compounds in the chromatographically analyzed samples according to the predominant chemical class

Class of compound	Fruits			Leaves		
	No. of peaks	Area / %		No. of peaks	Area / %	
		Hexane	Ethanol		Hexane	Ethanol
Acid	7	0.63	42.88	5	3.56	14.06
Alcohol	2	n.d.	1.70	8	4.74	19.11
Ester	14	1.41	20.68	10	7.04	8.29
Hydrocarbon	37	87.56	14.45	34	73.06	42.03
HMF (aldehyde)	1	n.d.	14.28	1	n.d.	8.08
Tocopherol	2	10.41	2.00	1	11.41	5.51
Others ^a	4	n.d.	4.02	10	0.18	2.93
Total	67	100	100	69	100	100

^aPhenols, aldehydes and ketones. The major compound classes are in bold.